

# Geometry of Chemical Graphs: Polycycles and Two-faced Maps

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# Preface

We study here two new, interesting for applications, especially, in Chemistry and Crystallography, classes of maps (on sphere or torus) generalizing Platonic polyhedra. *Polycycles* are 2-connected plane graphs having unique combinatorial type of interior faces and the same degree  $q$  for interior vertices, while at most  $q$  for boundary vertices. *Two-faced maps* are the maps, having at most two types of faces and the same degree of vertices.

We are interested mainly in enumeration, symmetry, extremal properties, face-regularity, metric embedding and related algorithmic problems.

The lists of graphs in this book come from broad areas of Geometry, Graph Theory, Chemistry and Crystallography. Many new interesting spheres and tori are presented.

The book is organised as follows. Chapters 1 and 2 give main notions. After reading them, each other chapter can be read almost independently.

Chapters 4–8 present theory of polycycles. In Chapter 4, we explain the general notion of  $(r, q)$ -polycycle, present the cases where classification is possible and the cell-homomorphism into the regular tiling  $\{r, q\}$ . In Chapter 5, the problem how the boundary of an  $(r, q)$ -polycycle determines it, or not, is addressed. In Chapter 6, we consider the possible symmetries of  $(r, q)$ -polycycles and how one can classify those with a symmetry group transitive on faces and/or vertices.

Chapter 7 presents a way to decompose a generalized polycycle into elementary components. This very pervasive technique is used in Chapters 8, 12, 13, 14 and 18.

The second main subject -  $k$ -valent two-faced maps - is treated in Chapters 3 and 9–19. Chapter 3 deals with our main example, fullerenes, while Chapter 9 classify strictly face-regular maps on sphere or torus. In Chapters 10–18, we consider a weaker notion of face-regularity. Chapter 19 treats 3-valent two-faced maps with icosahedral symmetry.

Many simple questions (some, possibly, easy) are raised; we hope that this book will be instrumental in their solution. Much of the results have been obtained and could only be obtained through computer enumeration; the corresponding programs are available from [Du07].

We are grateful to many people for their help with this book, especially, to Jacques Beigbeder, Gunnar Brinkmann, Olaf Delgado Friedrichs, Maja Dutour Sikirić, Patrick Fowler, Jack Graver, Marie Grindel, Viatcheslav Grishukhin, Stanislav Jendrol and Mikhail Shtogrin.

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# Chapter 1

## Introduction

In this chapter we introduce some basic definitions for graphs, maps and polyhedra. We present here basic notions, further definitions will be introduced later when needed. The reader can consult the following books for more detailed information: [Grü67], [Cox73], [Mun71], [Cro97].

### 1.1 Graphs

A *graph*  $G$  consists of a set  $V$  of *vertices* and a set  $E$  of *edges* such that each edge is assigned two vertices as its ends. Two vertices are *adjacent* if there is an edge between them. The *degree of a vertex*  $v \in V$  is the number of edges to which it is incident. A graph is said to be *simple* if no two edges have identical end-vertices. In the main special case of simple graphs, automorphisms are permutations of the vertices preserving adjacencies. For non-simple graphs (for example, when 2-gons occur) an *automorphism* of a graph is a permutation of the vertices and a permutation of the edges preserving incidence between vertices and edges. By  $\text{Aut}(G)$  is denoted the group of automorphisms of the graph  $G$ ; a synonym is *symmetry group*.

For  $U \subseteq V$ , let  $E_U \subseteq E$  be the set of edges of a graph  $G = (V, E)$  having both end-vertices in  $U$ . Then the graph  $G_U = (U, E_U)$  is called the *induced subgraph* (by  $U$ ) of  $G$ .

A graph  $G$  is said to be *connected* if, for any two of its vertices  $u, v$ , there is a path in  $G$  joining  $u$  and  $v$ . Given an integer  $k \geq 2$ , a graph is said to be *k-connected*, if it is connected and, after removal of any set of  $k - 1$  vertices, it remains connected.

Let  $G_1 = (V_1, E_1)$  and  $G_2 = (V_2, E_2)$  be two graphs. Their *Cartesian product*  $G_1 \times G_2$  is the graph  $G = (V_1 \times V_2, E)$  with vertex-set:

$$V_1 \times V_2 = \{(v_1, v_2) : v_1 \in V_1 \text{ and } v_2 \in V_2\}$$

and whose edges are the pairs  $((u_1, u_2), (v_1, v_2))$ , where  $u_1, v_1 \in V_1$  and  $u_2, v_2 \in V_2$ , such that either  $(u_1, v_1) \in E_1$ , or  $(u_2, v_2) \in E_2$ .

A subset  $E'$  of edges of a graph is called a *matching* if no two edges of  $E'$  have a common end-vertex. A *perfect matching* is a matching such that every vertex belongs to exactly one edge of the matching.

The following graphs will be frequently used:

- The *complete graph*  $K_n$  is the graph on  $n$  vertices  $v_1, \dots, v_n$  with  $v_i$  adjacent to  $v_j$  for all  $i \neq j$ .

- The *path*  $P_n = P_{v_1, v_2, \dots, v_n}$  is the graph with  $n$  vertices  $v_1, \dots, v_n$  and  $n - 1$  edges  $(v_i, v_{i+1})$  for  $1 \leq i \leq n - 1$ .
- The *circuit*  $C_n = C_{v_1, v_2, \dots, v_n}$  (or *n-gon*) is the path  $P_{v_1, v_2, \dots, v_n}$  with additional edge  $(v_1, v_n)$ .

A *plane graph* is a connected graph, together with an embedding on the plane such that every edge corresponds to a curve and no two curves intersect. A graph is *planar* if it admits at least one such embedding. Tutte ([Tut63]) proved that any planar graph admits a plane embedding with the edges being straight lines. A *face* of a plane graph is a part of the plane delimited by a circuit of edges. A plane graph defines a partition of the plane into faces. If  $a$  is a vertex, edge or face and  $b$  is a edge, face or vertex, then  $a$  is said to be *incident* to  $b$  if  $a$  is included in  $b$  or  $b$  is included in  $a$ . Two vertices, respectively, faces are called *adjacent* if they share an edge. We will call *gonality* of a face the number of its vertices. A face is *exterior* if it is non-bounded. Bounded faces are called *interior*. Any finite plane graph has exactly one exterior face. An infinite plane graph can have any number, from zero to an infinity, of exterior faces. A planar 3-connected graph admits exactly one plane embedding, i.e., the set of faces is determined by the edge-set.

The *v-vector*  $v(G) = (\dots, v_i, \dots)$  of a graph  $G$  enumerates the numbers  $v_i$  of vertices of degree  $i$ . A plane graph is *k-valent* if  $v_i = 0$  for  $i \neq k$ . The *p-vector*  $p(G) = (\dots, p_i, \dots)$  of a plane graph  $G$  counts the numbers  $p_i$  of faces of gonality  $i$ . For a connected plane graph  $G$ , denote its *plane dual graph* by  $G^*$  and define it on the set of faces of  $G$  with two faces being adjacent if they share an edge. Clearly,  $v(G^*) = p(G)$  and  $p(G^*) = v(G)$ .

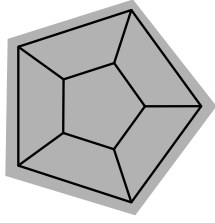
## 1.2 Topological notions

We present in this section the topological notions for surfaces which will be used. Topology is concerned with continuous structures and invariants under continuous deformations. Since we are working with vertices, edges, and faces, the classical definitions will be adapted to our context.

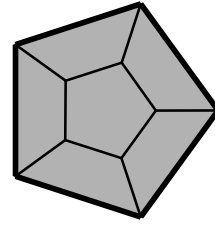
No proofs are given but we hope to compensate it by giving some geometrical examples. More thorough explanations are available in basic Algebraic Topology textbooks, for example, [Hat01] and [God71].

### 1.2.1 Maps

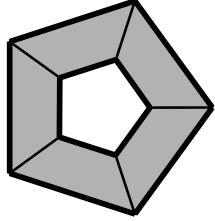
A *map*  $M$  is a family of vertices, edges and faces such that every edge is contained in at least one and at most two faces. An edge, contained in exactly one face, is called *boundary edge*; all such edges form the *boundary*. A map is called *closed* if it has no boundary. A map is called *finite* if it has a finite number of vertices, edges and faces. See below plane graphs related to  $Prism_5$  (see Section 1.5) with same vertex- and edge-sets but different face-sets; their boundary edges are boldfaced:



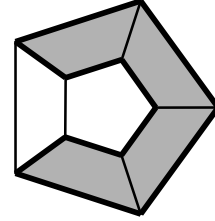
A closed map, cell-complex of a polyhedron. It is a  $5R_0, 4R_2$  plane graph (see Chapter 9).



A map with boundary edges. It is a  $(\{4, 5\}, 3)$ -polycycle (see Chapter 7).



A map with boundary edges; not simply connected. It is a  $(4, 3)_{gen}$ -polycycle (see Section 4.5).



Not a map because two edges are not contained in a face. It is not considered.

If  $M$  is a closed map, then one can define its dual map  $M^*$  by interchanging faces and vertices. See Section 4.1 for some related duality notions for non-closed maps. A map is called a *cell-complex* if the intersection of any two faces, edges, vertices is a face, edge, vertex or  $\emptyset$ . The maps with 2-gons are not cell-complexes; they are CW-complexes (see, for example, [Ro88]).

Denote by  $\mathbb{S}^2$  the 2-dimensional sphere defined by  $\{x = (x_1, x_2, x_3) \in \mathbb{R}^3 : x_1^2 + x_2^2 + x_3^2 = 1\}$ . For a point  $A$  of  $\mathbb{S}^2$ , let  $A'$  be its opposite and the plane  $\mathcal{H}_A$  is the plane orthogonal to  $AA'$  passing by  $A'$ . In the following, take  $A = (0, 0, -1)$ ; then  $\mathcal{H}_A$  is the set of all  $x \in \mathbb{R}^3$  with  $x_3 = 1$ . If  $B \in \mathbb{S}^2 - \{A\}$ , then the intersection of the line  $AB$  with the plane  $\mathcal{H}_A$  defines a point  $f_A(B)$ . This establish a bijection, called *Riemann map*, between  $\mathbb{S}^2 - \{A\}$  and the plane  $\mathcal{H}_A$ ; one can extend  $f_A$  to  $A$  by defining  $f_A(A)$  to be the “point at infinity” of the plane  $\mathcal{H}_A$ .

Let  $G$  be a finite plane graph on  $\mathbb{R}^2 \simeq \mathcal{H}_A$  and let  $f_A^{-1}(G)$  denote its image in  $\mathbb{S}^2$ . The vertices of  $G$  correspond to points of the sphere  $\mathbb{S}^2$ , the edges of  $G$  correspond to non-intersecting curvilinear lines on  $\mathbb{S}^2$  and the faces of  $G$  correspond to domains of  $\mathbb{S}^2$  delimited by circuit of those lines. The exterior face of  $G$  corresponds to a domain of  $\mathbb{S}^2$  containing  $A$ . Reciprocally, if one has a map  $M$  on the sphere, then one can find a point  $A$ , which does not belong to  $M$  and the corresponding plane  $\mathcal{H}_A$ , the image of  $M$  on  $\mathcal{H}_A$  is a finite plane graph. So, by abuse of language, we will use the term “sphere” not only for the surface  $\mathbb{S}^2$  but also for any combinatorial map on it, i.e., a finite plane graph.

A reader, who is interested only in plane graphs, our main subject, can move now directly to Section 1.4. But, for full understanding of the toric case, one needs maps in all their generality. For reference on Map Theory; see, for example, [BoLi95] and [Mo01].

We will also work with maps having an infinite number of vertices, edges and faces. The vertex-degrees will always be bounded by some constant; however, faces could have an infinity of edges. Amongst plane drawing of those maps, we will allow only the *locally finite* ones, i.e., those admitting an embedding such that any bounded domain contains

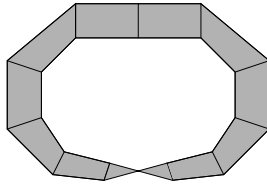


Figure 1.1: A Möbius strip

a finite number of vertices. Consider, for example, the map  $\widetilde{\mathbb{Z}^2}$  obtained as the quotient map of square tiling  $\mathbb{Z}^2$  by the translation operation  $(x, y) \mapsto (x + 10, y)$ . The map  $\widetilde{\mathbb{Z}^2}$  is an infinite cylinder made of consecutive rings of ten 4-gons. One can draw those rings concentrically on the plane, but the resulting plane graph will not be locally finite.

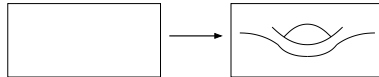
### 1.2.2 Orientability and classification of surfaces

A *flag of a map* is a triple  $(v, e, f)$ , where  $v$  is a vertex contained in the edge  $e$  and  $e$  is contained in the face  $f$ . Above condition allows to define three partially defined operators  $\sigma_0$ ,  $\sigma_1$  and  $\sigma_2$ , which maps a flag  $F = (v, e, f)$  to the unique other flag differing with  $F$  only in  $v$ ,  $e$  or  $f$ , respectively. Those operators  $\sigma_i$  act on the flag-set  $\mathcal{F}(M)$  of  $M$ . The operators  $\sigma_i$  are defined on every flag  $f \in \mathcal{F}(M)$  if and only if  $M$  is closed.

The map  $M$  is called *oriented* if there exist a bipartition  $\mathcal{F}_1, \mathcal{F}_2$  of  $\mathcal{F}(M)$  such that, for any  $(v, e, f) \in \mathcal{F}_1$ , the flag  $\sigma_i(v, e, f)$ , if it exists, belongs to  $\mathcal{F}_2$ . We will be almost exclusively concerned with oriented maps.

The notion of orientation is easy to define algebraically but difficult to visualize, because closed non-orientable maps cannot be represented by a picture. Fortunately, this is easier for maps with boundary; see on Figure 1.1 a non-orientable map, called *Möbius strip*. The non-orientability can be seen in the following way: moving on one side of the strip and doing a full circuit, one arrives on the other side of the strip. All boundary edges of a Möbius strip belong to a unique cycle; after adding a face on this cycle, one obtains the *projective plane*  $\mathbb{P}^2$ . The projective plane can also be obtained by taking a map on the sphere (like Dodecahedron) and identifying the opposite vertices, edges, faces, i.e., taking the *antipodal quotient*.

Given a surface  $S$ , one can add to it an *handle*:



or a *cross-cap*<sup>1</sup>. Handle and cross-cap can be seen as cylinder and Möbius strip, respectively.

Consider now the classification of finite maps:

**Theorem 1.2.1** *Any finite closed map is one of the following ones:*

1. the sphere  $\mathbb{S}^2$  (orientable),
2. the sphere  $\mathbb{S}^2$  with  $g$  handles (orientable),

---

<sup>1</sup>See, for example, <http://mathworld.wolfram.com/Cross-Cap.html> for pictures of cross-caps.

3. the sphere  $\mathbb{S}^2$  with  $g$  cross-caps (non-orientable).

Theorem 1.2.1 is proved, for example, in [Mun71]. The number  $g$  above is called the *genus* of the map. All finite closed maps, that occur below, are:

1. the sphere  $\mathbb{S}^2$  with  $g = 0$  (orientable),
2. the torus  $\mathbb{T}^2$  with  $g = 1$  (orientable),
3. the projective plane  $\mathbb{P}^2$  with  $g = 1$  (non-orientable),
4. the Klein bottle  $\mathbb{K}^2$  with  $g = 2$  (non-orientable); one way to obtain Klein bottle is to take the quotient of a torus  $\mathbb{R}^2/\mathbb{Z}^2$  by the fixed-point-free automorphism  $f(x, y) = (x + \frac{1}{2}, -y)$ .

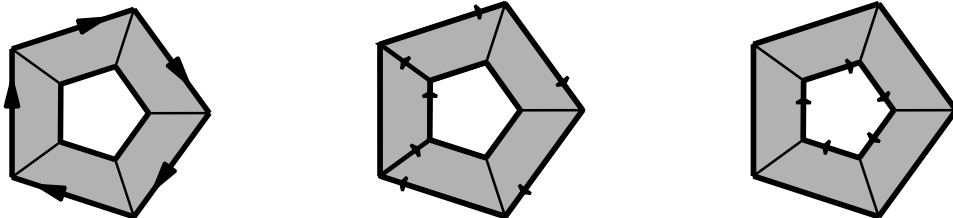
If  $M$  is a finite non-closed map, then one can add some faces along the boundary edges and obtain a closed map. So, finite non-closed maps are obtained by removing some faces of closed ones.

### 1.2.3 Fundamental groups, coverings and quotient maps

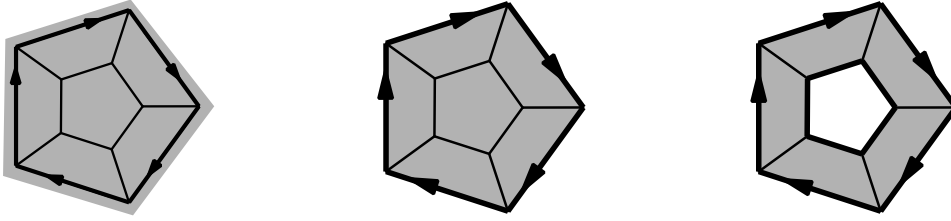
Fix an orientation on every edge of a given map  $M$  and define the free group  $G(\mathcal{M})$  with generators  $g_e$  indexed by the edge-set of  $M$  (see, for example, [Hu96] for relevant definitions in Group Theory). An *oriented path*  $\mathcal{OP}$   $v_1, v_2, \dots, v_m$  is a sequence of vertices with  $v_i$  adjacent to  $v_{i+1}$ . For an edge  $e_i = (v_i, v_{i+1})$ , denote by  $g(v_i, v_{i+1})$  the group element  $g_{e_i}$ , if  $e_i$  is oriented from  $v_i$  to  $v_{i+1}$  and  $g_{e_i}^{-1}$ , otherwise. Associate to the oriented path the product  $g(\mathcal{OP}) = g(v_1, v_2)g(v_2, v_3) \dots g(v_{m-1}, v_m)$ .

Denote by  $\mathcal{Z}_v(M)$  the set of all  $g(\mathcal{OP})$  with  $\mathcal{OP}$  being the set of oriented closed paths starting and finishing at a given *base vertex*  $v$ . It is a group; reversing orientation corresponds to taking inverse and product to concatenating closed paths. Given a face  $F$  of  $M$ , bounded by a circuit of vertices  $(v_1, \dots, v_{|F|})$ , and an oriented path  $\mathcal{OP}$  from the vertex  $v$  to the vertex  $v_1$ , consider a group element  $g(\mathcal{OP})g(v_1, v_2, \dots, v_{|F|}, v_1)g(\mathcal{OP})^{-1}$ . Denote by  $\mathcal{B}_v(M)$  the subgroup of  $G(\mathcal{M})$  generated by all such elements. The *fundamental group*  $\pi_1(M)$  is the quotient group of the group  $\mathcal{Z}_v(M)$  by the normal subgroup  $\mathcal{B}_v(M)$ . Two oriented closed paths having a common vertex  $v$  are called *homotopic* if they correspond to the same element in the group  $\pi_1(M)$ . The group  $\mathcal{B}_v(M)$  is the group of all elements homotopic to the *null path*, i.e., the path from  $v$  to  $v$  with 0 edges. If one replaces the base vertex  $v$  by another base vertex  $w$ , then, for any oriented path  $\mathcal{OP}$  from  $v$  to  $w$ , one has  $\mathcal{Z}_v(M) = g\mathcal{Z}_wg^{-1}$  and  $\mathcal{B}_v(M) = g\mathcal{B}_wg^{-1}$  with  $g = g(\mathcal{OP})$ . So, the fundamental group depends on the base vertex, but only up to conjugacy. A map is called *simply connected* if  $\pi_1(M)$  is trivial, i.e., every path is homotopic to the null path. This is equivalent to say that every two paths with same beginning and end can be continuously deformed one to the other.

See below three homotopic paths in the same map:



See below again three plane maps and a closed path represented in it:



$M_1$  is simply connected       $M_2$  is simply connected       $M_3$  is not simply connected

In  $M_1$  and  $M_2$ , the closed path is homotopic to a null path. In  $M_1$ , this cycle is the boundary of a face, while in  $M_2$ , the closed path is the boundary of all faces put together. More generally, a plane graph and a finite plane graph minus a face are simply connected. But the closed path in  $M_3$  is not homotopic to a null path. Actually, this closed path is a generator of the fundamental group  $\pi_1(M_3) \simeq \mathbb{Z}$ .

Given two maps  $M$  and  $M'$ , a *cell-homomorphism of maps*  $\phi : M \rightarrow M'$  is a function that maps vertices, edges, faces of  $M$  to the ones of  $M'$ , while preserving the incidence relations. An *isomorphism* is a cell-homomorphism, which is bijective. If  $M = M'$ , it is called an *automorphism*; the set of all automorphism of a map  $M$  is called the *symmetry group* of  $M$ . An automorphism  $f$  of a map  $M$  is called *fixed-point-free* if,  $f$  is the identity or for every vertex, edge, face of  $M$ , its image by  $f$  is different from it. If  $G$  is a group of fixed-point-free automorphisms of a map  $M$ , then  $M/G$  is the *quotient map* of  $M$  by  $G$ . Its vertices, edges and faces are formed by orbits of vertices, edges and faces of  $M$  (by  $G$ ) with the incidence relations being induced by the ones of  $M$ .

The quotient of a map can be very singular. Consider, for example, the 4-valent square tiling  $\{4, 4\}$  (see Section 1.5) formed by 4-gons and the group  $\mathbb{Z}^2$  acting by translations on it. There is one orbit of vertices, two orbits of edges and one orbit of faces under  $\mathbb{Z}^2$ ; so, the quotient  $\{4, 4\}/\mathbb{Z}^2$  is a torus represented by a single vertex and two loops.

For a vertex  $v$  (or edge  $e$ , or face  $f$ ), the *standard neighborhood*  $N(v)$  is the set of all vertices, edges and faces incident to  $v$ . A *local isomorphism* is a continuous mapping  $\phi : M \rightarrow M'$  such that, for any vertex  $v \in M$  (or edge, or face), the mapping from  $N(v)$  to  $N(\phi(v))$  is bijective. A *covering* is a local isomorphism such that for every vertex  $v' \in M'$  (or edge, or face) and  $w' \in N(v')$ , if  $\phi^{-1}(v') = (v_i)_{i \in I}$ , we have an element  $w_i \in N(v_i)$  such that  $w_i \neq w_j$  if  $i \neq j$  and  $\phi^{-1}(w') = (w_i)_{i \in I}$ .

If  $\mathcal{OP}' = (v'_1, \dots, v'_m)$  is an oriented path in  $M'$ ,  $\phi$  is a covering and  $v_1$  is a vertex in  $M$  with  $\phi(v_1) = v'_1$ , then there exists a unique oriented path  $\mathcal{OP} = (v_1, \dots, v_m)$  in  $M$  such that  $\phi(\mathcal{OP}) = \mathcal{OP}'$ . A *deck automorphism* is an automorphism  $u$  of  $M$  such that  $\phi \circ u = \phi$ ,  $u$  is necessarily fixed-point-free. If  $v' \in M'$ , then for any two  $v_1, v_2 \in \phi^{-1}(v')$ , there exists a deck automorphism  $u$  such that  $u(v_1) = v_2$ .

Given a map  $M$ , its *universal cover* is a simply connected map  $\widetilde{M}$  (unique up to isomorphism) with a covering  $\phi : \widetilde{M} \rightarrow M$ . The map  $\widetilde{M}$  is finite if and only if  $M$  and  $\pi_1(M)$  are finite. The fundamental group  $\pi_1(M)$  is isomorphic to the group of deck automorphisms of  $\phi$ . If  $H$  is a subgroup of a group  $G$ , then its *normalizer*, denoted by  $N_G(H)$ , is defined as:

$$N_G(H) = \{x \in G : xhx^{-1} \in H \text{ for all } h \in H\}.$$

The group  $\text{Aut}(M)$  of automorphisms of  $M$  is identified with the quotient group:

$$N_{\text{Aut}(\widetilde{M})}(\pi_1(M))/\pi_1(M).$$

The simplest and most frequently used case is when  $M$  is a closed finite map on the sphere. In this case  $\pi_1$  is trivial and one can represent the map nicely on the plane with a face chosen to be exterior. An infinite locally finite closed simply connected map can be represented on the plane. In this case, there is no exterior face and the map fills completely the plane.

A closed torus  $M$  can be represented as a 3-dimensional figure projected on the plane but this is not very practical. We represent its universal cover  $\widetilde{M}$  as a plane having two periodicity directions, i.e., a *2-periodic plane graph*. The group  $\pi_1(M)$  is isomorphic to  $\mathbb{Z}^2$  and it is represented on  $\widetilde{M}$  as a group of translation symmetries.

By choosing a *finite index subgroup*  $H$  of the group  $G$  (i.e., such that there exist  $g_1, \dots, g_m \in G$  with  $G = \cup_i g_i H$ ) of deck transformations and taking the quotient, one can obtain a bigger torus; such tori have a translation subgroup which is isomorphic to the quotient  $G/H$ .

On the other hand, given a torus with non-trivial translation group, there exists a unique *minimal torus* with the same universal cover and trivial translation subgroup. Those minimal tori correspond, in a one-to-one way, to periodic tilings of the plane.

### 1.2.4 Homology and Euler-Poincaré characteristic

Given a map  $M$ , assign an orientation on each of its edges and form a  $\mathbb{Z}$ -module  $C_1(M)$  using this set of oriented edges as basis. This  $\mathbb{Z}$ -module  $Z_1(M)$  is the submodule of  $C_1(M)$  generated by the set of closed cycles of  $M$ . Given any face of  $M$ , associate to it the set of incident edges in clockwise orientation; the generated  $\mathbb{Z}$ -module is denoted by  $B_1(M)$ . It is easy to see that  $B_1(M)$  is a submodule of  $Z_1(M)$ .

The *homology group*  $H_1(M)$  is the quotient of  $Z_1(M)$  by its subgroup  $B_1(M)$ . Again, we refer to Algebraic Topology textbooks for details. If  $M$  is a torus, then  $H_1(M)$  is isomorphic to  $\pi_1(M)$ .

If  $M$  is an orientable finite closed map, then  $H_1(M)$  is isomorphic to  $\mathbb{Z}^{2g}$ , where  $g$  is the genus of  $M$ . The *Euler-Poincaré characteristic* of a finite map  $M$  is defined as  $\chi(M) = v - e + f$  with  $v$  the number of vertices,  $e$  the number of edges and  $f$  the number of faces.

**Theorem 1.2.2** *For a finite closed map  $M$  of genus  $g$  it holds:*

- (i) *if  $M$  is orientable, then  $\chi(M) = 2 - 2g$ ,*
- (ii) *if  $M$  is non-orientable, then  $\chi(M) = 2 - g$ .*

This theorem is the main reason why we are able to use topology in dimension two to derive non-trivial combinatorial results.

**Theorem 1.2.3** *Let  $G$  be a  $k$ -valent closed map on a surface  $M$ ; then it holds:*

- (i) *The following Euler formula is valid:*

$$\sum_{j \geq 2} p_j(2k - j(k - 2)) = 2k\chi(M) \quad (1.1)$$

where  $p_i$  is the number of  $i$ -gonal faces.

- (ii) *If  $G$  has no 2-gonal faces, then  $k \leq 5$  if  $M$  is a sphere and  $k \leq 6$  if  $M$  is a torus.*

**Proof.** (i) The relation  $2e = kv$  allow us to rewrite the Euler-Poincaré characteristic as

$$\chi(M) = \left(\frac{2}{k} - 1\right)e + \sum_{i \geq 2} p_i.$$

Using that  $2e = \sum_{i \geq 2} ip_i$  in the above equation, yields the result.

If  $j \geq 3$ , then  $2k - j(k - 2) \leq 0$  for  $k \geq 6$  and  $2k - j(k - 2) < 0$  for  $k \geq 7$ . Assertion (ii) is deduced by noticing that  $\chi = 2, 0$  for sphere, torus, respectively.  $\square$

## 1.3 Representation of maps

A *polytope*  $P$  is the convex hull of a finite set of points in  $\mathbb{R}^n$ ; its *dimension* is the dimension of the smallest affine space containing it. We assume it to be full-dimensional. A linear inequality  $f(x) \geq 0$  is called *valid* if it holds for all  $x \in P$ . A *face* of  $P$  is a set of the form  $\{x \in P : f(x) = 0\}$  with  $f \geq 0$  being a valid inequality.

We will consider only 3-dimensional polytopes; they are called *polyhedra*. Their 0-dimensional faces are called *vertices* and the 2-dimensional faces are called just *faces*. Two vertices are called *adjacent* if there exist an *edge*, i.e., a 1-dimensional face containing both of them. The *skeleton* of a polyhedron is the graph formed by all its vertices with two vertices being *adjacent* if they share an edge. This graph is 3-connected and admits a plane embedding.

Given a polyhedron  $P$ , its skeleton  $skel(P)$  is a planar graph. Furthermore, for any face  $F$  of  $P$ , one can draw  $skel(P)$  on the plane so that  $F$  is the exterior face of the plane graph. Those drawings are called *Schlegel diagrams* (see, for example, [Zie95]). Steinitz (see [Ste22], [Zie95, Chapter 4] and [Grü03] for a clarification of the history of this theorem) proved that a finite graph is the skeleton of a polyhedron (and so, an infinity of polyhedra with the same skeleton) if and only if it is planar and 3-connected.

A *Riemann surface* is a 2-dimensional compact differentiable surface, together with an infinitesimal element of length (see textbooks on differential and Riemannian geometry, for example, [Na90]). The *curvature*  $K(x)$  at a point  $x$  is the coefficient  $\alpha$  in the expansion:

$$Vol(D(x, r)) = \pi r^2 - \alpha r^4 + o(r^4)$$

with  $D(x, r)$  being the disc consisting of elements at distance at most  $r$  from  $x$ . The curvature of a Riemann surface  $S$  satisfies the *Gauss-Bonnet formula*:

$$\int_S K(x) dx = 2\pi(1 - g).$$

All Riemann surfaces, considered in this section, will be of constant curvature. If a surface has constant curvature, then, for any two points  $x$  and  $y$  of it, there exist two neighborhoods  $N_x$  and  $N_y$  and a local isometry  $\phi$  mapping  $x$  to  $y$  and  $N_x$  to  $N_y$ . Hence, Riemann surfaces of constant curvature do not have local invariants and the only invariants they have are global (see, for example, [Jos06]). For genus zero, the curvature has positive integral. Up to rescaling, one can assume that this curvature is 1. There is only one such Riemann surface: the sphere  $\mathbb{S}^2$ . For genus 1, the curvature has integral 0 and so, it is 0. The Teichmüller space  $T_1$  has dimension 2, which means that Riemann surfaces of genus 1 are parametrized by two real parameters. Geometrically, they are very easy to

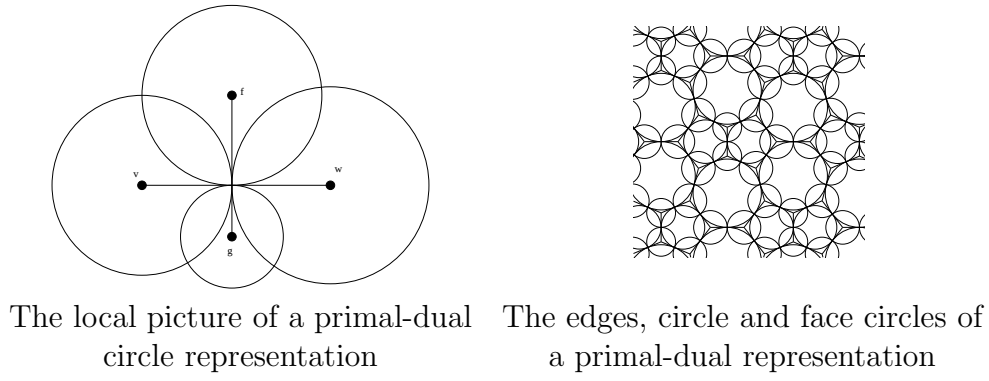


Figure 1.2: Illustration of primal-dual circle representations

depict: take  $\mathbb{R}^2$  and quotient it by a group  $v_1\mathbb{Z} + v_2\mathbb{Z}$ . For higher genus, the number of real parameters is  $6g - 6$  but we will not need them.

Given a map  $M$ , its *circle-packing representation* (see [Moh97]) is a set of disks on a Riemann surface  $\Sigma$  of constant curvature, one disk  $D(v, r_v)$  for each vertex  $v$  of  $M$ , such that the following conditions are fulfilled:

1. the interior of disks are pairwise disjoint,
2. the disk  $D(u, r_u)$ ,  $D(v, r_v)$  touch if and only if  $uv$  is an edge of  $M$ .

Simultaneous circle-packing representations of a map  $M$  and its dual  $M^*$  are called *primal-dual circle representation* of  $M$  if it holds:

1. If  $e = (u, v)$  is an edge of  $M$  and  $u^*$ ,  $v^*$  are the corresponding vertices in  $M^*$ , then the disks  $D(u, r_u)$ ,  $D(v, r_v)$  corresponding to  $e$ , touch at the same point as the disks  $D(u^*, r_{u^*})$ ,  $D(v^*, r_{v^*})$ .
2. The disks  $D(u, r_u)$ ,  $D(u^*, r_{u^*})$  cross at that point perpendicularly.

See on Figure 1.2 an illustration of this feature and an example of a primal-dual circle representation.

A map  $M$  is called *reduced* (see [Moh97, Section 3]) if its universal cover is 3-connected and is a cell-complex. It is shown in [Moh97, Corollary 5.4] that reduced maps admit unique primal-dual circle packing representations on a Riemann surface of the same genus; moreover, a polynomial time algorithm allows to find the coordinates of those points relatively easily. It means that the combinatorics of the map determines the structure of the Riemann surface.

The primal-dual representations allow us to get the uniqueness of the representation of given map. But, actually, for finite plane graphs, i.e., spheres, we use the program **CaGe** ([BDDH97]), which does not apply primal-dual representation. **CaGe** draws a Schlegel diagram of the plane, which we consider (see, Subsection 1.2.1); sometimes, in order to show the symmetry, it is a good idea to put one vertex or edge of the graph to infinity (see, for example, Figure 2.1, Section 9.1, Chapter 10).

For tori, we take their universal covers on the plane and use the primal-dual representation (see [Dut04]). For the projective plane  $\mathbb{P}^2$ , we take its universal cover, which is the sphere, and draw a circular frame, where antipodal boundary points are to be identified (see Figure 3.1). For the Klein bottle  $\mathbb{K}^2$ , we draw a rectangle with boundary identifications (see Figure 3.1).

## 1.4 Symmetry groups of maps

For finite closed maps on the sphere, there is a complete classification of possible symmetry groups. For finite closed maps on the torus, one can describe the possible symmetry groups of their universal covers.

Remind that an *automorphism* of a simple graph is a permutation of the vertices preserving adjacencies between vertices. For plane graphs, we require also that faces are sent to faces but for 3-connected graphs, this condition is redundant. Recall that  $Aut(G)$  denotes the group of automorphisms of  $G$ .

The *automorphism group*  $Aut(P)$  of a polyhedron  $P$  is the group of isometries preserving  $P$ . This group of isometries  $Aut(P)$  of a polyhedron  $P$  is a subgroup of the group of symmetries  $Aut(G)$  of the plane graph (the skeleton) of  $P$ . Mani [Man71] proved that any 3-connected plane graph  $G$  is the skeleton of at least one polyhedron  $P$  with  $Aut(G) = Aut(P)$ . So, one can identify the polyhedron and its skeleton, as well as the algebraic (permutation) symmetry group and the geometric (isometry) point group. For closed maps on surfaces of genus  $g > 0$ , one can use the primal-dual representation of the preceding section to prove that the symmetry group of the map can be realized as isometry group of the surface.

A *point group* is a finite subgroup of the group  $O(3)$  of isometries of the space  $\mathbb{R}^3$ , fixing the origin. Those groups have been classified a long time ago. They are described, for example, in [FoMa95], [Dut1] using the Schoenflies notation, which is used here (for the Hermann-Mauguin notation, see [OKHy96, Chapter 3], [Dut]). Every symmetry group of a finite plane graph is identified with a point group.

The list of point groups is split into two classes: seven infinite families and seven sporadic cases. Every point group contains a normal subgroup formed by its elements which are rotations.

We now list the infinite series of point groups:

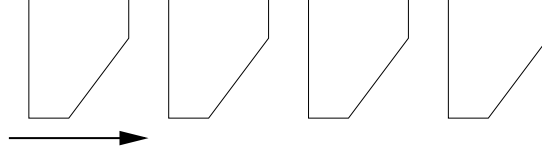
1. The group  $C_m$  is the cyclic group of rotations by angle  $\frac{2\pi}{m}k$  with  $0 \leq k \leq m - 1$  around a fixed axis  $\Delta$ .
2. The group  $C_{mh}$  is generated by  $C_m$  and a symmetry of plane  $P$  with  $P$  being orthogonal to  $\Delta$ .
3. The group  $C_{m\nu}$  is generated by  $C_m$  and a symmetry of plane  $P$  with  $P$  containing  $\Delta$ .
4. The group  $D_m$  is generated by  $C_m$  and a rotation by angle  $\pi$ , whose axis is orthogonal to  $\Delta$ .
5. The group  $D_{mh}$  is generated by  $C_{m\nu}$  and a rotation by angle  $\pi$ , whose axis is orthogonal to  $\Delta$  and contained in a plane of symmetry.
6. The group  $D_{md}$  is generated by  $C_{m\nu}$  and a rotation by angle  $\pi$ , whose axis is orthogonal to  $\Delta$  and going between two planes of symmetry.
7. For any even positive integer  $m$ , the group  $S_m$  is the cyclic group generated by the composition of a rotation by angle  $\frac{2\pi}{m}$  with axis  $\Delta$  and a symmetry of plane  $P$  with  $P$  being orthogonal to  $\Delta$ .

The particular cases  $C_1$ ,  $C_s = C_{1h} = C_{1v}$  and  $C_i = S_2$  correspond to the *trivial group*, the *plane symmetry group* and the *central symmetry inversion group*, respectively.

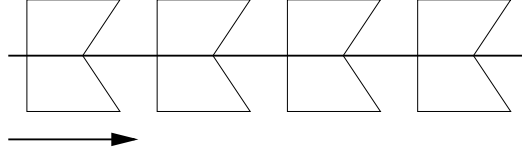
The point groups  $T_d$ ,  $O_h$  and  $I_h$  are the respective symmetry group of Tetrahedron, Cube and Icosahedron; the point groups  $T$ ,  $O$  and  $I$  are their respective normal subgroup of rotations. The point group  $T_h$  is formed by all  $f$  and  $-f$  with  $f \in T$ .

We now list the *strip groups* (also called *frieze groups*); this part follows [Cla, Dut]. There are also seven of them, since every such group corresponds to one of the infinite series of symmetry groups of plane graphs (imagine a graph of symmetry  $C_m, \dots, S_m$  and let  $m$  go to infinity, the figure become a strip):

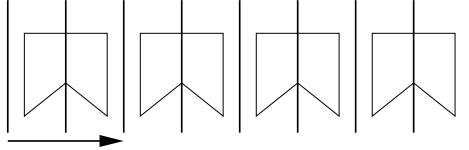
1.  $p111 (=C_\infty)$ ; it has only translational symmetry:



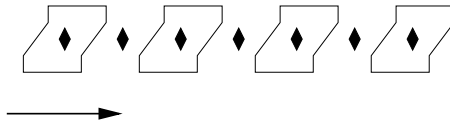
2.  $p1m1 (=C_{\infty h})$ ; it has a horizontal mirror symmetry:



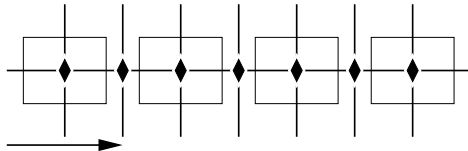
3.  $pm11 (=C_{\infty v})$ ; it has vertical mirror symmetries:



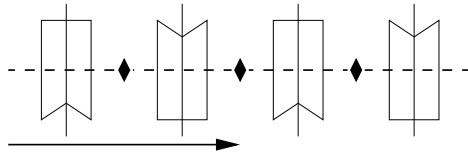
4.  $p112 (=D_\infty)$ ; it has only 2-fold rotations, spaced at half the translation distance:



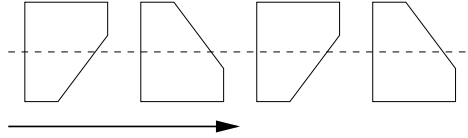
5.  $pmm2 (=D_{\infty h})$ ; it has vertical mirror symmetries, horizontal mirror symmetry and 2-fold rotations where the mirror intersect:



6.  $pma2 (=D_{\infty d})$ ; it has a glide reflections, with alternating vertical mirror and 2-fold rotations:

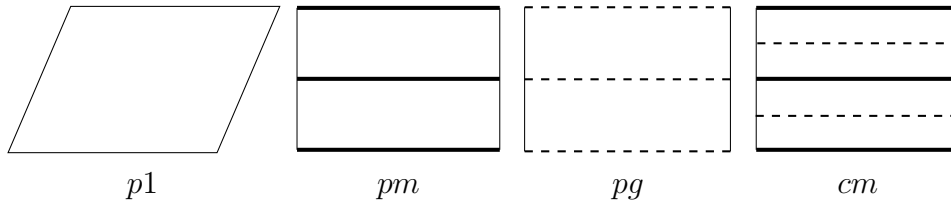


7.  $p1a1$  ( $=S_\infty$ ); it has glide reflections, half the length of the translation distance:

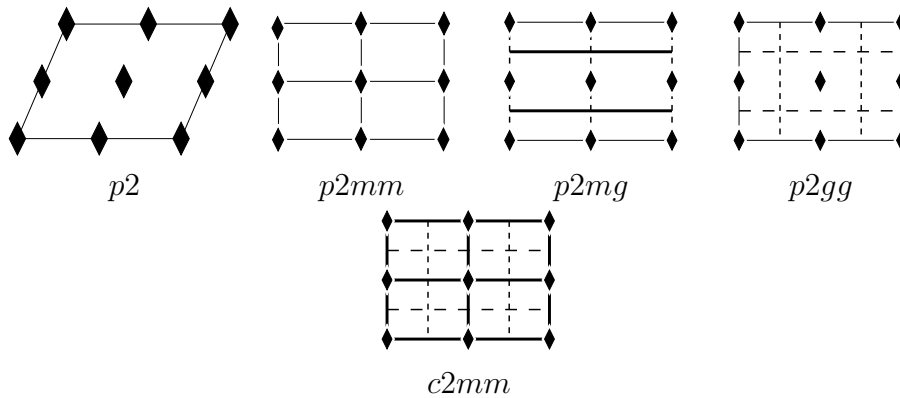


For 2-periodic plane maps, there are 17 possible symmetry groups, called *wallpaper groups* (or *plane crystallographic groups*), which are organized in five families (see, for example, [OKHy96, Chapter 1]):

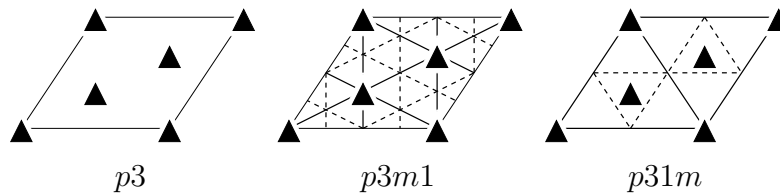
1. Wallpaper groups without rotations:



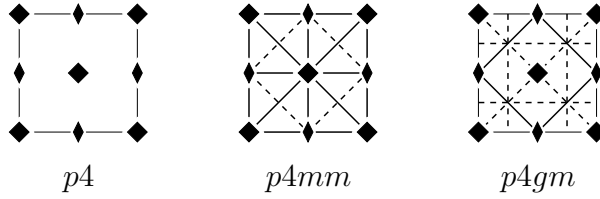
2. Wallpaper groups with rotations of order 2:



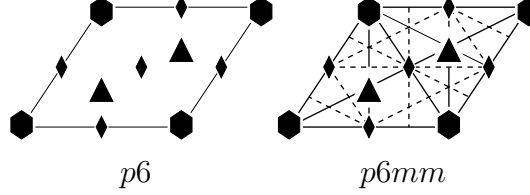
3. Wallpaper groups with rotations of order 3:



4. Wallpaper groups with rotations of order 4:



5. Wallpaper groups with rotations of order 6:



Consider now 2-dimensional *Coxeter groups* (see, for example, [Cox73, Hu96]). By  $T^*(l, m, n)$  is denoted a Coxeter *triangle group*. It is defined abstractly as the group with generators  $a, b, c$  and relations:

$$a^2 = b^2 = c^2 = 1 \text{ and } (ab)^l = (ac)^m = (bc)^n = 1.$$

Denote by  $\alpha(l, m, n)$  the number  $\frac{1}{l} + \frac{1}{m} + \frac{1}{n} - 1$ .

The group  $T^*(l, m, n)$  can be realized as a group of isometries of a simply connected surface  $X$  of constant curvature, where:

- $X = \mathbb{S}^2$ , i.e., the 2-dimensional sphere, if  $\alpha(l, m, n) > 0$ ,
- $X = \mathbb{R}^2$ , i.e., the Euclidean plane, if  $\alpha(l, m, n) = 0$ ,
- $X = \mathbb{H}^2$ , i.e., the hyperbolic plane, if  $\alpha(l, m, n) < 0$  (see [Cox98]).

For a group  $G$  acting on a surface  $X$ , a *fundamental domain* is a closed set  $\mathcal{D}$ , the orbit of which under  $G$  tiles  $X$ , i.e., every point belongs to at least one image of  $\mathcal{D}$  under  $G$  and the intersection of any two domains in the orbit have empty interior. For the group  $T^*(l, m, n)$  acting on  $X$ , one can find a fundamental domain, which is a triangle  $ABC$ , so that  $a, b$  and  $c$  are reflections along the sides  $BC, AC, AB$ . The angles at  $A, B$  and  $C$  are, respectively,  $\frac{\pi}{n}, \frac{\pi}{m}$  and  $\frac{\pi}{l}$ .

The integral of the curvature over the triangle  $ABC$  is  $\pi\alpha(l, m, n)$ . If  $X = \mathbb{S}^2$  of curvature 1, then the area of the triangle is  $\pi\alpha(l, m, n)$ . If  $X = \mathbb{H}^2$  of curvature  $-1$ , then the area of the triangle is  $-\pi\alpha(l, m, n)$ . If  $X = \mathbb{R}^2$  of curvature 0, then the area of the triangle is not determined by  $\alpha(l, m, n)$ .

If  $\alpha(l, m, n) > 0$  (*elliptic case*), then  $T^*(l, m, n)$  is a finite group acting on the sphere  $\mathbb{S}^2$ ; the only possibilities for  $(l, m, n)$  are:

1.  $(2, 2, n)$  for  $n \geq 2$  with  $T^*(2, 2, n) \simeq D_{nh}$  being the automorphism group of the regular  $n$ -gon,
2.  $(2, 3, 3)$  with  $T^*(2, 3, 3) \simeq T_d$  being the automorphism group of Tetrahedron,
3.  $(2, 3, 4)$  with  $T^*(2, 3, 4) \simeq O_h$  being the automorphism group of Octahedron,
4.  $(2, 3, 5)$  with  $T^*(2, 3, 5) \simeq I_h$  being the automorphism group of Icosahedron.

If  $\alpha(l, m, n) = 0$  (*parabolic case*), then  $T^*(l, m, n)$  is a wallpaper group acting on the plane  $\mathbb{R}^2$ ; the only possibilities for  $(l, m, n)$  are:

1.  $(2, 4, 4)$  with  $T^*(2, 4, 4) \simeq p4mm$  being the automorphism group of the square tiling  $\mathbb{Z}^2$  of  $\mathbb{R}^2$ ,
2.  $(2, 3, 6)$  with  $T^*(2, 3, 6) \simeq p6mm$  being the automorphism group of the triangular tiling of  $\mathbb{R}^2$ .

If  $\alpha(l, m, n) < 0$  (*hyperbolic case*), then there is an infinity of possibilities for  $(l, m, n)$ .

By  $T(l, m, n)$  is denoted the normal subgroup of index two of  $T^*(l, m, n)$  formed by rotations of  $X$  (i.e., orientation-preserving elements of  $T^*(l, m, n)$ ); see, for example, [Mag74].

There are following relations with strip groups:

$$T^*(2, 2, \infty) = pmm2 \text{ and } T(2, 2, \infty) = p112 \approx pm11 \approx pma2.$$

Remark that  $p1m1$  also has index two in  $T^*(2, 2, \infty)$ , but it is not isomorphic to  $T(2, 2, \infty)$ . Recall also that  $T(2, 3, \infty) \approx PSL(2, \mathbb{Z})$  (the *modular group*) and  $T^*(2, 3, \infty) \approx SL(2, \mathbb{Z})$ . The groups  $T(l, m, n)$  contain a large number of non-isomorphic subgroups of finite index which renders futile any hope of classification of possible symmetry groups of maps on orientable surfaces of genus  $g \geq 2$ . However, in many cases considered here, the groups  $T(l, m, n)$  and  $T^*(l, m, n)$  are sufficient for our purposes.

**Remark 1.4.1** In Chapters 2, 4 and 7, a pair  $(r, q)$  will be called elliptic, parabolic, hyperbolic if  $rq < 2(r + q)$ ,  $rq = 2(r + q)$ ,  $rq > 2(r + q)$ , respectively. This is equivalent to  $\alpha(2, r, q) > 0$ ,  $\alpha(2, r, q) = 0$ ,  $\alpha(2, r, q) < 0$ , respectively. In Chapter 4, the link will be made direct, since every  $(r, q)$ -polycycle has a cell-homomorphism into the tiling  $\{r, q\}$  (see Section 1.5), whose symmetry group is  $T^*(2, r, q)$ .

In Chapter 7, there will be no such link; however, the fact that  $(r, q)$  is elliptic will have strong structural consequences and, perhaps, a link can be found.

A  $k$ -valent sphere, whose faces have gonality  $a$  or  $b$  is called a  $(\{a, b\}, k)$ -sphere (see Chapter 2). We call the parameters  $(\{a, b\}, k)$  elliptic, parabolic, hyperbolic, according to the sign of  $\alpha(2, b, q)$ . This sign has as well strong consequences on the class of  $(\{a, b\}, k)$ -spheres (finiteness, growth, etc.). Here, the link is provided by Euler formula (1.1).

## 1.5 Types of regularities of maps

We list here some classification results for maps on the sphere or on the plane.

A map is *regular* if its automorphism group act *transitively* on flags, i.e., if, for any two flags  $f$  and  $f'$ , there is an automorphism  $\phi$  with  $\phi(f) = f'$ .

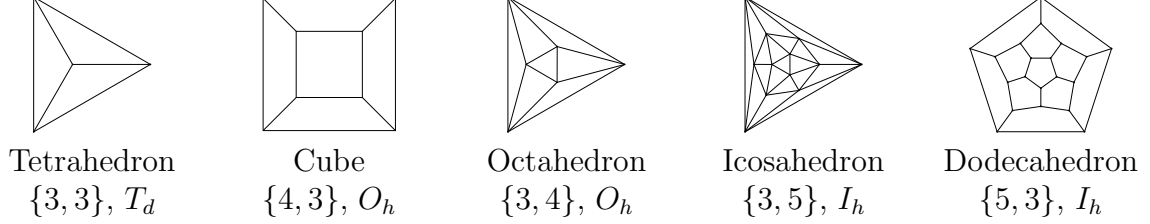
We are now in position to define formally the *regular tiling*  $\{r, q\}$ .

**Definition 1.5.1** The triangle group  $T^*(2, r, q)$  act on  $X$  (with  $X = \mathbb{S}^2, \mathbb{R}^2, \mathbb{H}^2$ ) if  $\alpha(2, r, q) > 0$ ,  $= 0$ ,  $< 0$ , respectively. The fundamental domain  $\mathcal{D}$  (triangle  $ABC$ ) has angles  $\frac{\pi}{q}$ ,  $\frac{\pi}{r}$  and  $\frac{\pi}{2}$  at  $A$ ,  $B$ ,  $C$ , respectively.

To every point  $B'$  in the orbit of  $B$  under  $T^*(2, r, q)$ , associate an  $r$ -gon formed by all  $2r$  triangles containing  $B'$ . The tiling  $\{r, q\}$  is the set of all those  $r$ -gons, it satisfies to:

- $\{r, q\}$  is a  $q$ -valent tiling of  $X$  by  $r$ -gons.
- The group  $T^*(2, r, q)$  act regularly on  $\{r, q\}$ , i.e., any two flags of  $\{r, q\}$  are equivalent under  $T^*(2, r, q)$ .
- the curvature of those  $r$ -gons is  $2r\alpha(2, r, q)$ .

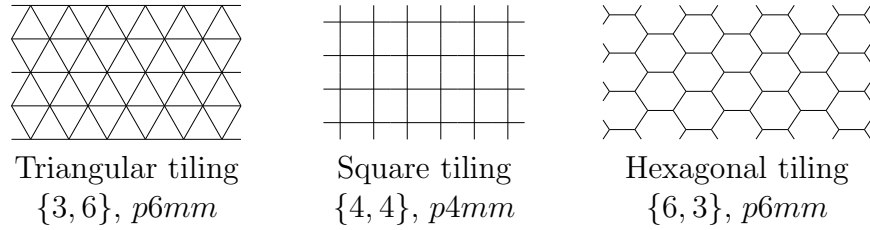
See below the Platonic (regular) polyhedra  $P$  with their groups  $Aut(P)$ :



One has the duality  $Cube = (Octahedron)^*$  and  $Icosahedron = (Dodecahedron)^*$ , while Tetrahedron is self-dual.

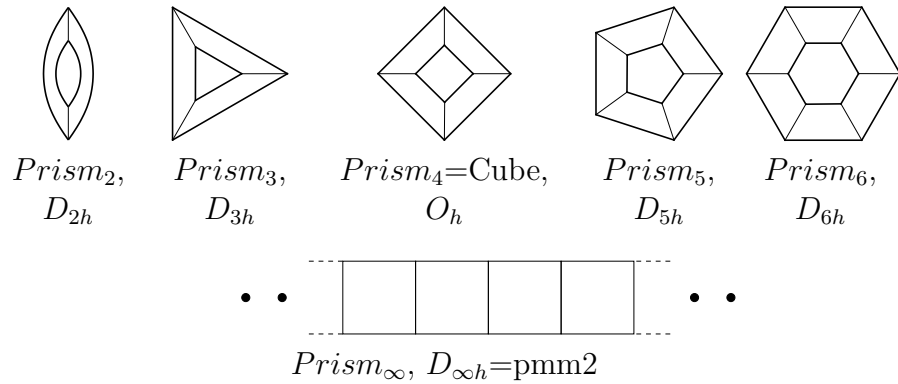
Denote by  $Bundle_m$ ,  $m \geq 2$ , the plane graph with two vertices and  $m$  edges between them (so,  $m$  2-gonal faces). The plane graph  $Bundle_m$ , which is dual to  $m$ -gon, has the symmetry group  $D_{mh} = T^*(2, 2, m)$  and it is a regular map, which is not a cell-complex.

Three regular tilings of the plane  $\mathbb{R}^2$  are:

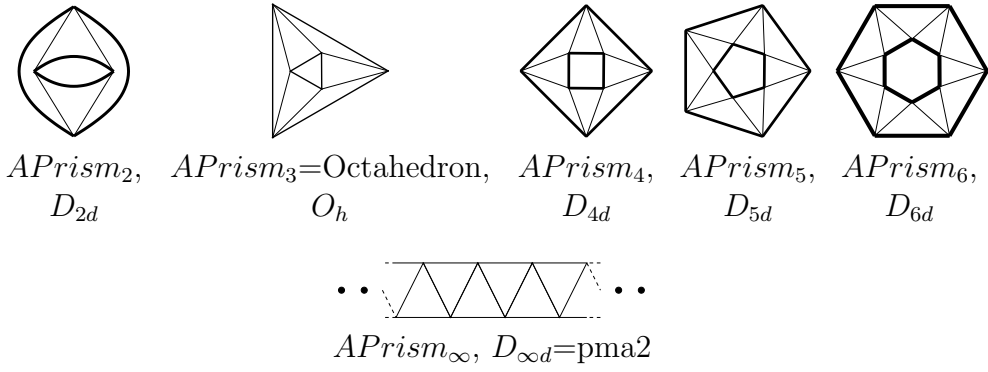


The triangular and hexagonal tilings are dual to each other, while the square tiling is self-dual. For other parameters  $(r, q)$ , the tiling  $\{r, q\}$  lives in hyperbolic space  $\mathbb{H}^2$  (see many pictures in [Eps00]) but we will not need it.

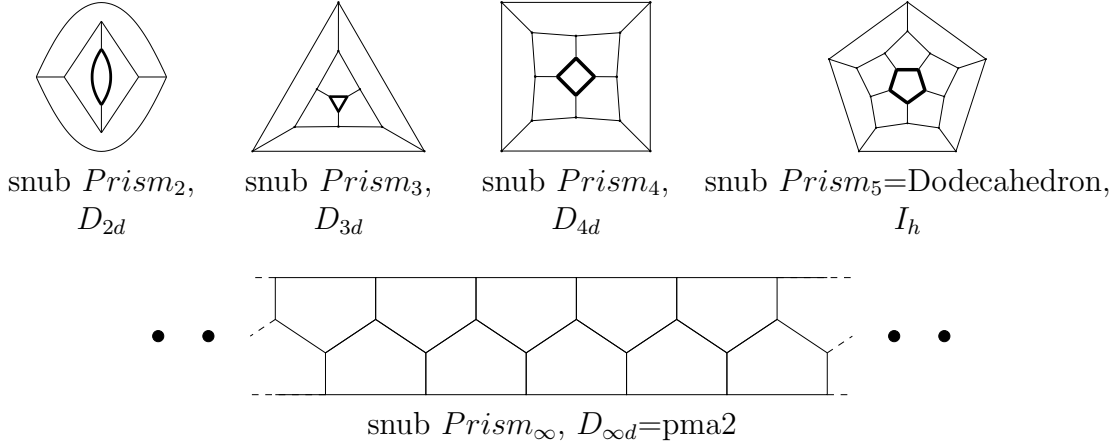
Given two circuits  $U = (u_1, \dots, u_m)$  and  $V = (v_1, \dots, v_m)$ , an  $Prism_m$  ( $m$ -sided prism), for  $2 \leq m \leq \infty$ , is a 3-valent plane graph, where each  $u_i$  is joined to  $v_i$  by an edge. Its symmetry group is  $D_{mh}$  if  $m \neq 4$  and  $O_h$  if  $m = 4$ .



An  $APrism_m$  ( $m$ -sided antiprism), for  $2 \leq m \leq \infty$ , is a 4-valent plane graph formed by adding to two circuits  $U$  and  $V$  the cycle  $(u_1, v_2, u_2, v_3, \dots, v_m, u_m, v_1, u_1)$ . Its symmetry group is  $D_{md}$  if  $m \neq 3$  and  $O_h$  if  $m = 3$ .

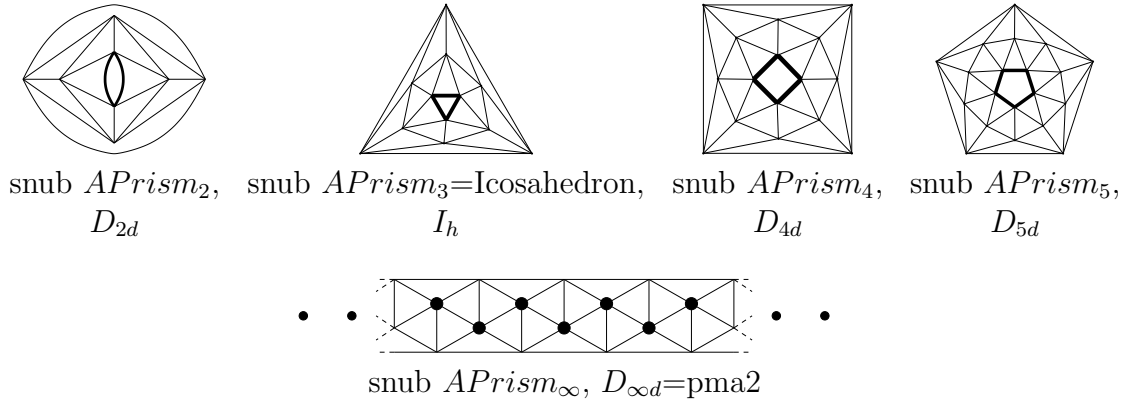


For  $2 \leq m \leq \infty$ , denote by *snub Prism<sub>m</sub>* a 3-valent plane graph with two  $m$ -gonal faces separated by two  $m$ -rings of 5-gons. Its symmetry group is  $D_{md}$  if  $m \neq 5$  and  $I_h$  if  $m = 5$ .



Snub *Prism<sub>3</sub>* is also called *Dürer octahedron* (see it on the painting *Melanholia* by Dürer, 1514, depicting the muse of Mathematics at work) and it can be obtained by truncating Cube on two opposite vertices.

For  $2 \leq m \leq \infty$ , denote by *snub APrism<sub>m</sub>* a 5-valent plane graph with two  $m$ -gonal faces separated by  $6m$  3-gonal faces as in examples below (see [DGS04, page 119], for formal definition). Its symmetry group is  $D_{md}$  if  $m \neq 3$  and  $I_h$  if  $m = 3$ .



Snub *APrism<sub>4</sub>* is one of 92 *regular-faced<sup>2</sup>* polyhedra called *snub square antiprism* (see [Joh66] and [Zal69]).

<sup>2</sup><http://mathworld.wolfram.com/JohnsonSolid.html>

A map is called *Archimedean* if its symmetry group acts transitively on vertices but the map itself is not regular. Any Archimedean polyhedron belongs either to 13 sporadic examples, or to one of two infinite series  $Prism_m$  and  $APrism_m$  for  $m \geq 3$ . Like the Platonic polyhedra, they are known since the antiquity and were rediscovered during the Renaissance; Kepler ([Kep1619]) gave them their modern names. Their duals are called *Catalan polyhedra*. The Archimedean tilings of the plane are also classified. There are eight such maps; their duals are called *Laves tilings*.

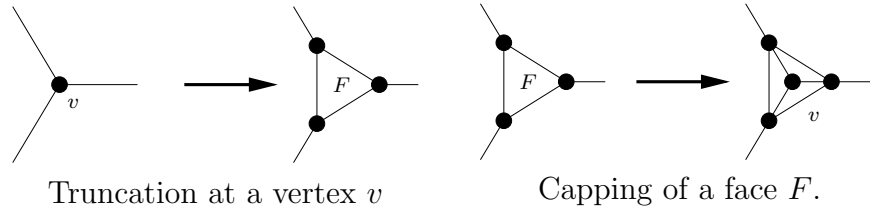
All 92 regular-faced polyhedra was found by the work of many people, especially, of Johnson and Zalgaller (see, for example, [Joh66, Zal69]). The eight ones (namely, Tetrahedron, Octahedron, Icosahedron and duals of  $Prism_3$  and four  $(\{4, 5\}, 3)$ -spheres from Figure 2.1), whose faces are regular triangles, are called *deltahedra*. A *mosaic* is a tiling of Euclidean plane by regular polygons. All (165) mosaics are classified in [Cha89].

## 1.6 Operations on maps

A *decorated*  $\{r, q\}$  is a map obtained by adding some edges to the regular tiling  $\{r, q\}$ ; see in Tables 9.1 and 9.3 many such decorations.

We list here some operations transforming a map  $M$  into another map  $M'$ .

**Truncation and capping:** The *truncation of  $M$  at a vertex  $v$*  of degree  $m$  consists of replacing the vertex  $v$  by a  $m$ -gonal face. The *capping* is, in a sense, dual to truncation, it consists of adding a new vertex  $v$  to a face  $F$  of  $M$  such that  $v$  is adjacent to all vertices of  $F$ , i.e., putting a pyramid on  $F$ .

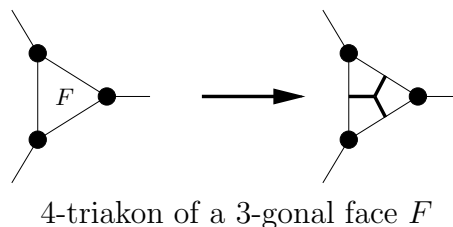


The *truncation of  $M$* , respectively, *capping of  $M$*  consist of doing truncation, respectively, capping of all vertices, respectively, faces of  $M$ . The *t-capping of  $M$*  is obtained by doing capping of  $t$  distinct faces of  $M$ . The *b-cap of  $M$*  is the map obtained by capping all  $b$ -gonal faces of  $M$ .

**Elongation:** Let  $C$  be a simple circuit of adjacent vertices in  $M$ . An *elongation of  $M$  along  $C$*  consists of replacing  $C$  by a ring of 4-gons (see a related notion of *central circuit* in Chapter 2). The elongation of  $M$  along a circuit  $C$ , bounding a face  $F$ , means adding a prism on  $F$ .

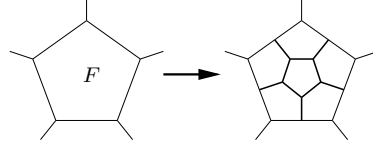
**$m$ -halving:** Given an even number  $m$ , a  *$m$ -halving of  $M$*  is obtained by putting new edge, connecting the mid-points of opposite edges, on each  $m$ -gon.

**4-triakon:** The *4-triakon of a 3-gonal face  $F$*  of  $M$  is obtained by partitioning  $F$  into three 4-gons according to the scheme below:



The 4-*triakon* of  $M$  consists of doing 4-triakon of all 3-gons of  $M$ .

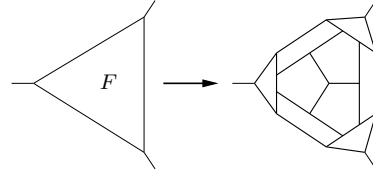
**Pentacon:** The *pentacon* of a 5-gonal face  $F$  of  $M$  consists of partitioning  $F$  into six 5-gons according to the scheme below:



Pentacon of a 5-gonal face  $F$ .

If  $S$  is a set of 5-gons of  $M$  such that no two 5-gons in  $S$  are adjacent, then denote by  $P_S(M)$  the *pentacon* of  $M$  on  $S$ , i.e., the pentacon of all 5-gons in  $S$ .

**5-triakon:** The 5-triakon of a 3-gonal face  $F$  of  $M$  consists of partitioning  $F$  into nine 5-gons according to the scheme below:



5-triakon of a 3-gonal face  $F$

Actually, the 3-gons to which we will apply this construction, come from the truncation of a set of vertices  $S$  of a map  $M$ . The result of this operation (truncation followed by 5-triakon of new 3-gonal faces) is denoted by  $T_S(M)$  and is called 5-*triakon* of  $M$  on  $S$ .

Remark that last two operations amount to replace a face by  $(5, 3)$ -polycycles  $A_5$ ,  $A_3$  (see Chapter 7 and Figure 7.2), respectively.

# Chapter 2

## Two-faced maps

Call a *two-faced map* and, specifically,  $(\{a, b\}, k)$ -map, any  $k$ -valent map with only  $a$ - and  $b$ -gonal faces, for given integers  $2 \leq a < b$ . We will also use terms  $(\{a, b\}, k)$ -sphere (moreover,  $(\{a, b\}, k)$ -polyhedron if it is 3-connected) or  $(\{a, b\}, k)$ -torus, for maps on sphere  $\mathbb{S}^2$  or torus  $\mathbb{R}^2$ , respectively. Call  $(\{a, b\}, k)$ -plane any infinite  $k$ -valent plane graph with  $a$ - and  $b$ -gonal faces and without exterior faces. More generally, for  $R \subset \mathbb{N} - \{1\}$ , call  $(R, k)$ -map a  $k$ -valent map, whose faces have gonalitys  $i \in R$ .

When presenting a  $(\{a, b\}, k)$ -sphere in a drawing, we will indicate its number of vertices and its Schoenflies symmetry group (see Section 1.4). The notation  $(v, p_a, p_b)$  under picture of a minimal  $(\{a, b\}, k)$ -torus indicates its number of vertices, its number of  $a$ - and  $b$ -gonal faces; we also indicate its wallpaper symmetry group (see Section 1.4).

Call *corona* (of a face) the sequence of gonalitys of all its consecutive neighbors. The *corona* of a vertex is the sequence of gonalitys of all consecutive faces containing it. Recall that  $v$ ,  $e$  and  $f$  denote the number of vertices, edges and faces, respectively, of a given finite map. Denote by  $p_i$  the number of its  $i$ -gonal faces and by  $e_{a-b}$ ,  $e_{a-a}$  the number of  $(a-b)$ -edges,  $(a-a)$ -edges, i.e., edges separating  $a$ - and  $b$ -gonal faces or, respectively,  $a$ -gonal faces. Euler Formulas (1.1) for  $(\{a, b\}, k)$ -sphere and  $(\{a, b\}, k)$ -torus are:

$$\begin{aligned} p_a(2k - a(k - 2)) + p_b(2k - (k - 2)b) &= 4k, \\ p_a(2k - a(k - 2)) + p_b(2k - (k - 2)b) &= 0. \end{aligned}$$

One can interpret the quantity  $2k - b(k - 2)$  as the curvature of the faces of gonality  $b$ ; Euler formula is the condition that the total curvature is a constant, equal to  $4k$ , for  $k$ -valent plane graphs. This curvature has an interpretation and applications in Computational Group Theory, see [Pa06] and [LySc77, Chapter 9].

A pair  $(R, k)$  is called *elliptic*, *parabolic*, *hyperbolic* if  $\frac{1}{r} + \frac{1}{k} > \frac{1}{2}$ ,  $= \frac{1}{2}$ ,  $< \frac{1}{2}$ , where  $r = \max_{i \in R} i$ , respectively.

The  $(\{5, 6\}, 3)$ -spheres are called *fullerenes* in Organic Chemistry, where fullerenes and other two-faced maps are prominent molecular models. The  $(\{5, 7\}, 3)$ -spheres are called, in chemical context, *azulenoids* (see Figure 7.1 for *azulene*).

The  $(\{a, b\}, k)$ -spheres with elliptic  $(\{a, b\}, k)$ , i.e., with  $b(k - 2) < 2k$ , are listed in Figure 2.1.

We will mainly consider in this chapter  $(\{a, b\}, k)$ -spheres with parabolic  $(\{a, b\}, k)$ , i.e., with  $2k = b(k - 2)$ ; for those, the number  $p_a$  of  $a$ -gonal faces remains fixed:

$$p_a = \frac{4k}{2k - a(k - 2)}.$$

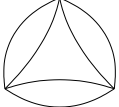
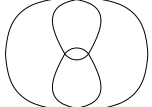
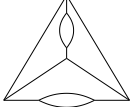
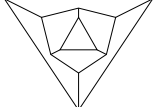
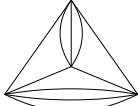
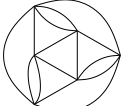
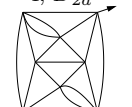
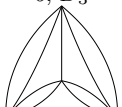
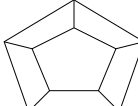
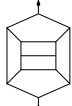
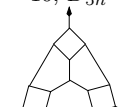
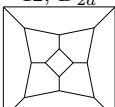
| $(\{a, b\}, k)$ | plane graphs                                                                                                                                                                                                                                                                                                                                                                                           | $(\{a, b\}, k)$ | plane graphs                                                                                                                                                                                                                                                                                                                                                                                                           |
|-----------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $(\{2, 3\}, 4)$ | <br>$3, D_{3h}$<br><br>$4, D_{2d}$                                                                                                                                                                                                   | $(\{2, 5\}, 3)$ | <br>$4, D_{2d}$                                                                                                                                                                                                                                                                                                                     |
| $(\{2, 4\}, 3)$ | <br>$4, D_{2h}$                                                                                                                                                                                                                                                                                                       | $(\{3, 5\}, 3)$ | <br>$12, D_{3d}$                                                                                                                                                                                                                                                                                                                    |
| $(\{2, 3\}, 5)$ | <br>$4, D_{2d}$<br><br>$6, D_3$<br><br>$8, D_2$<br><br>$4, D_{2d}$ | $(\{4, 5\}, 3)$ | <br>$10, D_{5h}$<br><br>$12, D_{2d}$<br><br>$14, D_{3h}$<br><br>$16, D_{4d}$ |

Figure 2.1: All  $(\{a, b\}, k)$ -spheres with elliptic  $(\{a, b\}, k)$  and  $p_b \geq 1$

In other words, every  $a$ -gonal face of  $G$  has positive curvature and every  $b$ -gonal face has zero curvature.

Is is easy to see that the only (seven) solutions are  $(\{a, b\}, k) = (\{2, 6\}, 3), (\{3, 6\}, 3), (\{4, 6\}, 3), (\{5, 6\}, 3), (\{2, 4\}, 4), (\{3, 4\}, 4)$  and  $(\{2, 3\}, 6)$ .<sup>1</sup>

If the number of vertices becomes large, then those plane graphs are formed by a few faces of gonality  $a$  in a sea of faces of gonality  $b$ . But there is a unique way to have  $k$ -valent tiling of the plane with faces of gonality  $b$ : the regular 2-periodic tiling  $\{b, k\}$  of  $\mathbb{R}^2$ . The case  $(\{5, 6\}, 3)$  of fullerenes alone created an entire industry (see [FoMa95]), first reference is [Gol35] and even reverend Kirkman, who studied in 1882 40-vertex fullerenes, was cited in [Gol35].

For the hyperbolic classes  $(\{a, b\}, k)$ , i.e., those with  $2k < b(k - 2)$ , (see [BCC96]), things are much more complicate. It is likely that the number of such graphs grows more than exponentially with increasing number  $v$  of vertices (the growth rate for them is unknown like many other things) and the combinatorics is so rich that it becomes intractable by the methods exposed here. But Malkevitch ([Mal70]) proved that 3-valent polyhedra, i.e.,  $(\{a, b\}, 3)$ -polyhedra with  $b \geq 7$ , exist, with finite number of exceptions, if and only if  $(6 - a)p_a - (b - 6)p_b = 12$ , i.e., Euler formula (1.1) holds. Moreover, he found:

- (i)  $b \in \{7, 8, 9, 10\}$ , if  $a = 3$ ,
- (ii)  $p_b$  is even, if  $2a$  divide  $b$  and  $a = 4, 5$ .

<sup>1</sup>We attributed before to those seven classes the following names and notation, respectively:  $2_v, 3_v, 4_v, 5_v$  (in [DeDu05]), 4-hedrites, octahedrites (in [DeSt03, DDS03, DHL02]),  $(2, 3)_v$ .

If  $p_b = 0$ , then the above seven possible classes of  $(\{a, b\}, k)$ -spheres with parabolic  $(\{a, b\}, k)$  give *Bundle*<sub>3</sub>, Tetrahedron, Cube, Dodecahedron, *Bundle*<sub>4</sub>, Octahedron and *Bundle*<sub>6</sub>, respectively (see definition of *Bundle*<sub>*m*</sub> in Section 1.5).

If  $p_b = 1$ , then such spheres do not exist.

Theorem 2.2.1 below gives that  $(\{2, 6\}, 3)$ -sphere with  $v$  vertices exists if and only if  $v = 2(k^2 + kl + l^2)$  for some integers  $0 \leq k \leq l$ .

Theorem 2 of [GrMo63] gives that a  $(\{3, 6\}, 3)$ -polyhedron with  $v$  vertices exists only for any  $v \geq 4$  with  $v \equiv 0 \pmod{4}$ , except of  $v = 8$ . For  $v = 8$ , a  $(\{3, 6\}, 3)$ -sphere exists but it is only 2-connected sphere  $T_1$ ; see Proposition 2.0.2.

The  $(\{4, 6\}, 3)$ -spheres were considered in a chemical setting in [GaHe93]. Theorem 1 of [GrMo63] gives that a  $(\{4, 6\}, 3)$ -sphere with  $v$  vertices exists only for any even  $v \geq 8$ , except  $v = 10$ .

Theorem 1 of [GrMo63] gives also that a  $(\{5, 6\}, 3)$ -sphere with  $v$  vertices exists only for any even  $v \geq 20$ , except  $v = 22$ .

A  $(\{2, 4\}, 4)$ -sphere with  $v$  vertices exists for any even  $v \geq 2$  (see [DeSt03]).

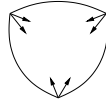
The existence of  $(\{3, 4\}, 4)$ -spheres with  $v$  vertices only for any  $v \geq 6$ , except  $v = 7$ , is established in [Grü67, page 282].

A  $(\{2, 3\}, 6)$ -sphere with  $v$  vertices exists for any  $v \geq 2$  and the proof (in the same spirit as for other parabolic classes) is given below.

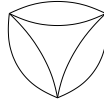
**Theorem 2.0.1** *For any  $v \geq 2$ , there exists a  $(\{2, 3\}, 6)$ -sphere.*

**Proof.** Consider the regular tiling  $\{3, 6\}$  and take the doubly infinite path  $l$  of vertices lying on a straight line in  $\{3, 6\}$ . If one take another parallel line  $l'$  at distance  $t$ , then  $l$  and  $l'$  bound a domain  $D_t$  in  $\{3, 6\}$ .

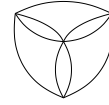
If one takes the group  $G$  generated by a translation of three edges along  $l$ , then the quotient  $\tilde{D}_t$  of  $D_t$  by  $G$  is formed of  $t$  rings, each of six 3-gons. The domain  $\tilde{D}_t$  has two faces bounded by vertices of degree 4. There are two possible caps to close those structures:



Incomplete structure

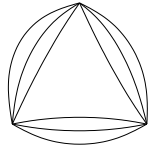


Cap Nr. 1

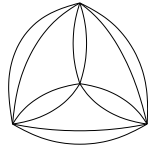


Cap Nr. 2.

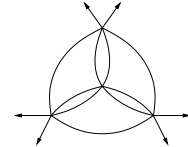
Denote by  $23_1(t)$  the  $(\{2, 3\}, 6)$ -sphere with  $3t + 3$  vertices, which is formed by closing domain  $\tilde{D}_t$  by two caps Nr. 1. Denote by  $23_2(t)$  the  $(\{2, 3\}, 6)$ -sphere with  $3t + 4$  vertices, which is formed by closing domain  $\tilde{D}_t$  by one cap Nr. 1 and one cap Nr. 2. Denote by  $23_3(t)$  the  $(\{2, 3\}, 6)$ -sphere with  $3t + 5$  vertices, which is formed by closing domain  $\tilde{D}_t$  by two caps Nr. 2. See below the first two members of those series:



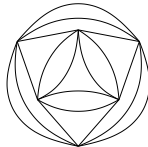
3,  $D_{3h}$  ( $23_1(0)$ )



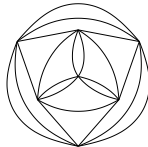
4,  $T_d$  ( $23_2(0)$ )



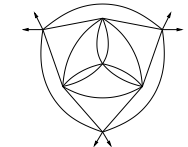
5,  $D_{3h}$  ( $23_3(0)$ )



6,  $D_{3d}$  ( $23_3(1)$ )



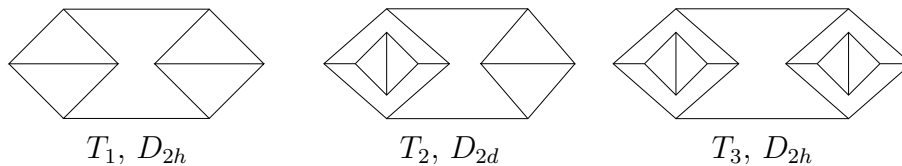
7,  $C_{3v}$  ( $23_2(1)$ )



8,  $D_{3d}$  ( $23_1(1)$ )

$Bundle_6$  has two vertices. □

Denote by  $(T_n)_{n \geq 1}$  the infinite series of  $4(n+1)$ -vertex  $(\{3, 6\}, 3)$ -spheres, whose first three members are shown below:



The symmetry group of  $T_n$  is  $D_{2d}$  or  $D_{2h}$  if  $n$  is even or odd, respectively.

**Theorem 2.0.2** ([DeDu05]) *For a 3-valent plane graph  $G$  with faces of gonality between 3 and 6, it holds:*

- (i)  $G$  is 2-connected.
- (ii) If  $G$  is not 3-connected, then it belongs to the infinite series  $T_n$  of  $(\{3, 6\}, 3)$ -spheres.

There is a similar theorem in [DDS03] for 4-valent plane graphs with faces of size 2, 3 or 4. From this it follows that  $(\{3, 4\}, 4)$ -,  $(\{4, 6\}, 3)$ - and  $(\{5, 6\}, 3)$ -spheres are polyhedra.

## 2.1 The Goldberg-Coxeter construction

The Goldberg-Coxeter construction takes a 3- or 4-valent plane graph  $G_0$ , two integers  $k$  and  $l$  and returns another 3- or 4-valent plane graph denoted by  $GC_{k,l}(G_0)$ . This construction occurs in a many contexts, whose (non-exhaustive) list (for the main case of  $G_0$  being Dodecahedron) is given below:

1. Every fullerene  $(\{5, 6\}, 3)$  of symmetry  $I$  or  $I_h$  is of the form  $GC_{k,l}(Dodecahedron)$  for some  $k$  and  $l$ , i.e., is parametrized by a pair of integers  $k, l \geq 0$ . This result was proved by Goldberg in [Gol37]; see some other proofs in [Cox71] and Theorem 2.2.2.
2. The famous fullerene  $C_{60}(I_h)$  (called *buckminsterfullerene* or *soccer ball*) has the skeleton of  $GC_{1,1}(Dodecahedron)$ .  $GC_{k,l}(Dodecahedron)$  constitute a particularly studied class of fullerenes (see [FoMa95, Diu03]).
3. A certain class of virus *capsides* (protein shells of virions) have a spherical structure, that is modeled on dual  $GC_{k,l}(Dodecahedron)$  (see [CaKl62, Cox71, DDG98]).
4. Geodesic domes, designed with the method of Buckminster Fuller, are based again on those two parameters  $k$  and  $l$  (see [Cox71]).
5. In Numerical Analysis on the sphere, one needs system of points that roughly looks uniform. The vertices of dual  $GC_{k,l}(Dodecahedron)$  provide such a point-set (see [ScSw95]).
6. Some conjectural solutions of many extremal problem on the sphere (Thomson, Tammes, Skyrme problems, etc.) have (solving exactly the problem is almost impossible) combinatorial structure of  $GC_{k,l}(Dodecahedron)$  or its dual (see [HaSl96]).

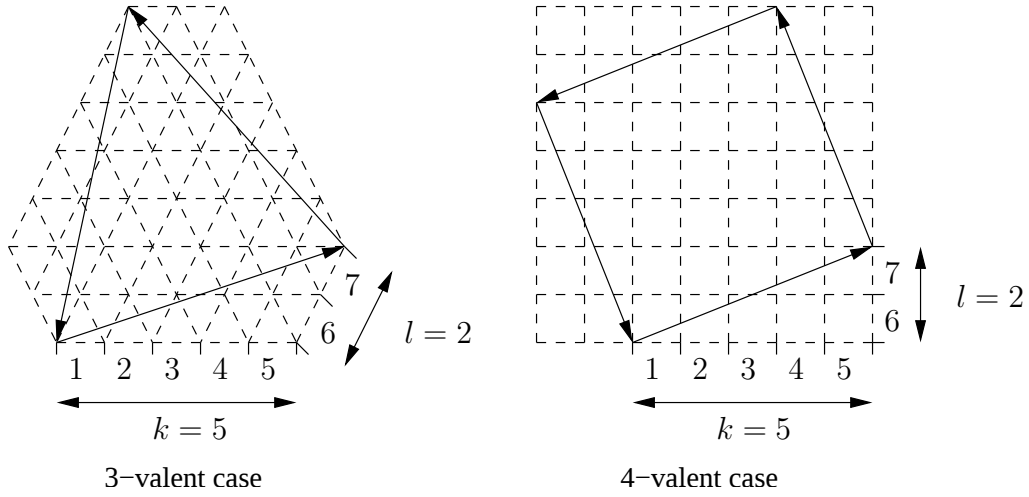


Figure 2.2: The master polygon in 3- or 4-valent case

In Virology, the number  $t(k, l) = k^2 + kl + l^2$  (used for icosahedral fullerenes) is called *triangulation number*. In terms of Buckminster Fuller, the number  $k+l$  is called *frequency*, the case  $l = 0$  is called *Alternate*, and the case  $l = k$  is called *Triacon*. He also called the Goldberg-Coxeter construction *Breakdown* of the initial plane graph  $G_0$ .

The *root lattice*  $A_2$  is defined by  $A_2 = \{x \in \mathbb{Z}^3 : x_0 + x_1 + x_2 = 0\}$ . The *square lattice* is denoted by  $\mathbb{Z}^2$ .

The ring  $\mathbb{Z}[\omega]$ , where  $\omega = e^{\frac{2\pi i}{6}} = \frac{1}{2}(1 + i\sqrt{3})$ , of *Eisenstein integers* consists of the complex numbers  $z = k + l\omega$  with  $k, l \in \mathbb{Z}$ . The norm of such  $z$  is denoted by  $N(z) = z\bar{z} = k^2 + kl + l^2$  and we will use the notation  $t(k, l) = k^2 + kl + l^2$ . If one identifies  $x = (x_1, x_2, x_3) \in A_2$  with the Eisenstein integer  $z = x_1 + x_2\omega$ , then it holds  $2N(z) = \|x\|^2$ .

The ring  $\mathbb{Z}^2 = \mathbb{Z}[i]$  consists of the complex numbers  $z = k + li$  with  $k, l \in \mathbb{Z}$ . The norm of such  $z$  is denoted by  $N(z) = z\bar{z} = k^2 + l^2$  and we will use the notation  $t(k, l) = k^2 + l^2$ .

The Goldberg-Coxeter construction for 3- or 4-valent plane graphs can be seen, in algebraic terms, as the scalar multiplication by Eisenstein or Gaussian integers in the parameter space. More precisely,  $GC_{k,l}$  corresponds to multiplication by complex number  $k + l\omega$  or  $k + li$  in the 3- or 4-valent case, respectively.

Let us now build the graph  $GC_{k,l}(G_0)$ . First consider the 3-valent case. By duality, every 3-valent plane graph  $G_0$  can be transformed into a *triangulation*, i.e., into a plane graph whose faces are triangles only. The Goldberg-Coxeter construction with parameters  $k$  and  $l$  consists of subdividing every triangle of this triangulation into another set of faces, called *master polygon*, according to Figure 2.2, which is defined by two integer parameters  $k, l$ . The obtained faces, if they are not triangles, can be glued with other non-triangle faces (coming from the subdivision of neighboring triangles), in order to form triangles. So, one ends up with a new triangulation (see Figure 2.3).

The triangle of Figure 2.2 has area  $\mathcal{A}(k^2 + kl + l^2)$  if  $\mathcal{A}$  is the area of a small triangle. By transforming every triangle of the initial triangulation in such way and gluing them, one obtains another triangulation, which we identify with a (dual) 3-valent plane graph and denote by  $GC_{k,l}(G_0)$ . The number of vertices of  $GC_{k,l}(G_0)$  (if the initial graph  $G_0$  has  $v$  vertices) is  $vt(k, l)$  with  $t(k, l) = k^2 + kl + l^2$ .

For a 4-valent plane graph  $G_0$ , the duality operation transforms it into a quadrangulation and this initial quadrangulation is subdivided according to Figure 2.2, which is also

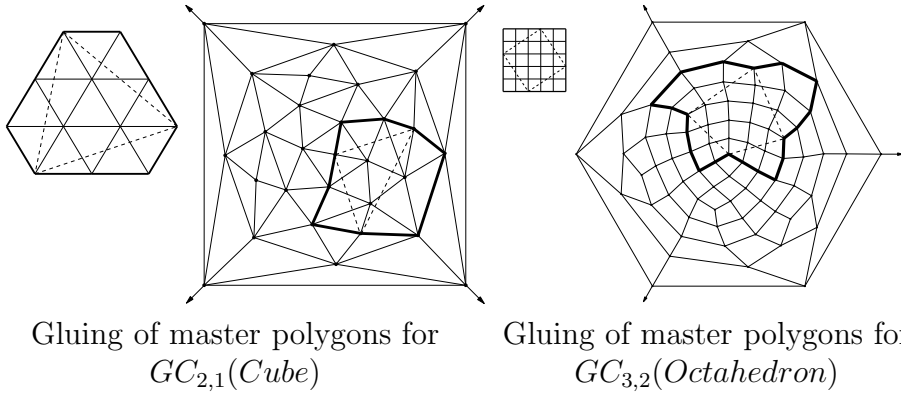


Figure 2.3: Two examples of gluing of master polygons

defined by two integer parameters  $k, l$ . After merging, the obtained non-square faces, one gets another quadrangulation and the duality operation yields the 4-valent plane graph  $GC_{k,l}(G_0)$  having  $nt(k, l)$  vertices with  $t(k, l) = k^2 + l^2$  (see Figure 2.3).

The faces of  $G_0$  correspond to some faces of  $GC_{k,l}(G_0)$ . If  $t(k, l) > 1$ , then those faces are not adjacent; they are isolated amongst 6-gons or 4-gons.

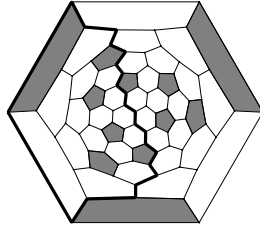
**Theorem 2.1.1** ([DuDe03]) *Let  $G_0$  be a 3- or 4-valent plane graph and denote the graph  $GC_{k,l}(G_0)$  also by  $GC_z(G_0)$ , where  $z = k + l\omega$  or  $z = k + li$  in 3- or 4-valent case, respectively. Then the following holds:*

- (i)  $GC_z(GC_{z'}(G_0)) = GC_{zz'}(G_0)$ .
- (ii) If  $z' = z\alpha^u$  with  $\alpha = \omega$  or  $i$ ,  $G_0$  is 3- or 4-valent and  $u \in \mathbb{Z}$ , then  $GC_z(G_0) = GC_{z'}(G_0)$ .
- (iii)  $GC_{\bar{z}}(G_0) = GC_z(\overline{G_0})$ , where  $\overline{G_0}$  denotes the plane graph, which differ from  $G_0$  only by a plane symmetry.

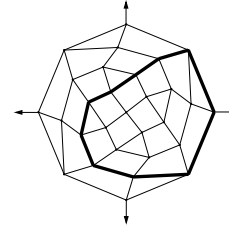
For a map  $G$ , denote by  $Med(G)$  its *medial map*. The vertices of  $Med(G)$  are the edges of  $G$ , two of them being adjacent if the corresponding edges share a vertex and belong to the same face of  $G$ . So,  $Med(G) = Med(G^*)$ . One has  $Med(Tetrahedron) = Octahedron$  and  $Med(Cube) = Cuboctahedron$ . The skeleton of  $Med(G)$  is the line graph of the skeleton of  $G$  if  $G$  is a 3-valent map.

For any 3-valent map  $G$ , the *leapfrog* of  $G$  is the truncation of  $G^*$  (see [FoMa95]). One can check that  $GC_{1,1}(G)$  is the leapfrog of  $G$ .

If  $l = 0$ , then  $GC_{k,l}(G_0)$  is called *k-inflation* of  $G_0$ . For  $k = 2, l = 0$ , it is called *chamfering* of  $G_0$ , because Goldberg called the result of his construction for  $(k, l) = (2, 0)$  on Dodecahedron, *chamfered Dodecahedron*. All symmetries of  $G$  occur in  $GC_{k,l}(G)$  if  $l = 0$  or  $l = k$ , while only rotational symmetries are preserved if  $0 < l < k$ . The Goldberg-Coxeter construction can be also defined, similarly, for maps on orientable surfaces. While the notions of medial, leapfrog and *k-inflation* go over for non-orientable surfaces, the Goldberg-Coxeter construction is not defined on a non-orientable surface. Some examples of Goldberg-Coxeter construction can be found in Chapter 9. It is interesting to study graph parameters of  $GC_{k,l}(G)$  for a fixed  $G$ ; one example of such study concerns *zigzags* and *central circuits* in [DuDe03].



Simple zigzag in a 88-vertex  
 $(\{5, 6\}, 3)$ -sphere,  $T$



Simple central circuit in a 30-vertex  
 $(\{3, 4\}, 4)$ -sphere,  $O$

Figure 2.4: Examples of simple zigzag and central circuit; one orbit of such 12 zigzags and one orbit of six such circuits

## 2.2 Description of the classes

Here are presented some known theoretical and computer tools for generating  $(\{a, b\}, k)$ -spheres. We first give the cases, for description of which the Goldberg-Coxeter construction suffices. Then, for  $(\{3, 6\}, 3)$ - and  $(\{2, 4\}, 4)$ -spheres simple combinatorial constructions give a full description of those classes. For the remaining classes, one has less possibilities and the number of graphs grows more sharply with increasing number of vertices.

**Theorem 2.2.1** *Every  $(\{2, 6\}, 3)$ -plane graph comes as  $GC_{k,l}(Bundle_3)$ ; its symmetry group is  $D_{3h}$  if  $l \in \{0, k\}$  and  $D_3$ , otherwise.*

**Proof.** The description of those spheres is given in [GrZa74] and it is, actually, Goldberg-Coxeter construction.  $\square$

**Theorem 2.2.2** (i) Any  $(\{3, 6\}, 3)$ -sphere with symmetry  $T$  or  $T_d$  is  $GC_{k,l}(Tetrahedron)$ ,  
(ii) any  $(\{4, 6\}, 3)$ -sphere with symmetry  $O$  or  $O_h$  is  $GC_{k,l}(Cube)$ ,  
(iii) any  $(\{4, 6\}, 3)$ -sphere with symmetry  $D_6$  or  $D_{6h}$  is  $GC_{k,l}(Prism_6)$ ,  
(iv) any  $(\{5, 6\}, 3)$ -sphere with symmetry  $I$  or  $I_h$  is  $GC_{k,l}(Dodecahedron)$ ,  
(v) any  $(\{2, 4\}, 4)$ -sphere with symmetry  $D_4$  or  $D_{4h}$  is  $GC_{k,l}(Bundle_4)$ ,  
(vi) any  $(\{3, 4\}, 4)$ -sphere of symmetry  $O$  or  $O_h$  is  $GC_{k,l}(Octahedron)$ .  
(vii) Let  $\mathcal{GP}_m$  (for  $m \neq 2, 4$ ) denote the class of 3-valent plane graphs with two  $m$ -gonal faces,  $m$  4-gons and  $p_6$  6-gonal faces. Every such graph, having a  $m$ -fold axis, comes as  $GC_{k,l}(Prism_m)$  and has symmetry group  $D_m$  or  $D_{mh}$ .  
(viii) Let  $\mathcal{GF}_m$  (for  $m \neq 2, 3$ ) denote the class of 4-valent plane graphs with two  $m$ -gonal faces,  $m$  2-gons and  $p_4$  4-gonal faces. Every such graph, having a  $m$ -fold axis, comes as  $GC_{k,l}(Foil_m)$  and has symmetry group  $D_m$  or  $D_{mh}$ .

The above results are proved in [Gol37, Cox71, DuDe03]. We will prove only (ii), the other cases being very similar: Take a  $(\{4, 6\}, 3)$ -sphere of symmetry  $O$  or  $O_h$ . One 4-fold symmetry axis goes through a 4-gon, say,  $F_1$ . After adding  $p$  rings of 6-gons around  $F_1$ , one finds a 4-gon and so, by symmetry, four 4-gons, say,  $F'_1, F'_2, F'_3, F'_4$ . The position of the square  $F'_1$  relatively to  $F_1$  defines an Eisenstein integer  $z = k + l\omega$ . The graph can be completed in a unique way and this proves, that it is  $GC_{k,l}(Cube)$ . Looking back at the proof one can see that we used only the existence of a 4-fold rotation axis to get the result.

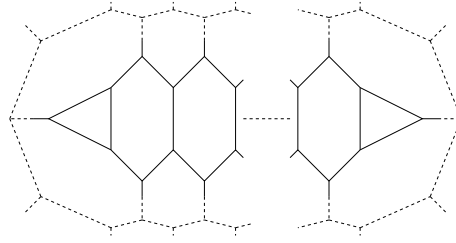
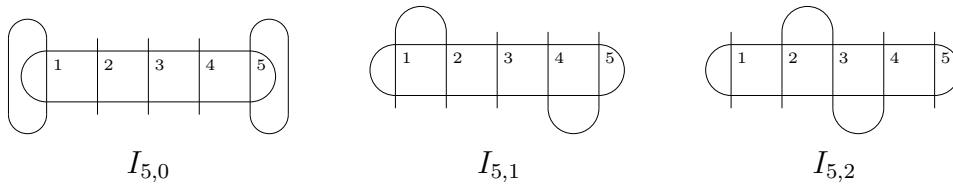


Figure 2.5: A railroad and a closed railroad in a  $(\{3, 6\}, 3)$ -sphere

Therefore, the symmetry group  $C_4$ ,  $D_4$  and so on are not possible for  $(\{4, 6\}, 3)$ -spheres, i.e., such symmetry implies some higher symmetries.

We are now giving the general construction of all  $(\{3, 6\}, 3)$ -spheres following [GrMo63] (see also [DeDu05]). A *zigzag* in a plane graph is a circuit of edges, such that any two, but no three, consecutive edges belong to the same face. A zigzag is called *simple* if it has no self-intersection (see, for example, Figure 2.6). A *closed railroad* in a 3-valent plane graph is a circuit of 6-gonal faces, such that any 6-gon is adjacent to its neighbors on opposite edges. A 3-valent plane graph is called *tight* if it has no closed railroads. A *railroad* between two non 6-gonal faces  $F$  and  $F'$  is a sequence of 6-gons, say,  $F_1, \dots, F_l$ , such that putting  $F_0 = F$  and  $F_{l+1} = F'$ , we have that any  $F_i$ ,  $1 \leq i \leq l$ , is adjacent to  $F_{i-1}$  and  $F_{i+1}$  on opposite edges. It is proved in [GrMo63] that closed railroads and railroads of a  $(\{3, 6\}, 3)$ -sphere do not self-intersect, i.e., a given 6-gon occur only once. Take a  $(\{3, 6\}, 3)$ -sphere  $G$ , a railroad between two triangles  $T_1, T_2$  and denote by  $s$  the number of 6-gons of this railroad. Around this structure, one adds rings of 6-gons, which happen to be closed railroads. After adding  $m$  such rings, one adds a triangle  $T_3$ . The structure is then completely determined and one obtains a railroad between  $T_3$  and  $T_4$ , which is isomorphic to the one between  $T_1$  and  $T_2$  (see Figure 2.5 for illustration). We get, by direct computation, the equality  $p_6 = 2(sm + s + m)$  and  $v = 4(s + 1)(m + 1)$ , where  $p_6$  is the number of 6-gons and  $v$  the number of vertices.

Following [DeSt03], we now explain how to describe all  $(\{2, 4\}, 4)$ -spheres. In a 4-valent graph, a *central circuit* is a circuit of edges such that any two consecutive edges are not contained in a common face (see Figure 2.4). A central circuit is called *simple* if it has no self-intersection. A central circuit is determined by a single edge, so the edge-set is partitioned by the central circuits. A *railroad* is a, possibly self-intersecting, circuit of 4-gons bounded by two central circuits. A 4-valent graph is called *tight* if it has no railroad. Non-tight 4-valent graphs are obtained from tight ones by duplicating some of its central circuits. It is proved that all central circuits of  $(\{2, 4\}, 4)$ -sphere do not self-intersect. Let us describe the tight  $(\{2, 4\}, 4)$ -spheres. They have exactly two central circuits. Below we indicate the starting point of the construction for  $v = 5$ :



From the scheme drawn above, it is clear that there is only one way of completing the structure so as to obtain a  $(\{2, 4\}, 4)$ -sphere, which we denote by  $I_{v,i}$ . Also  $I_{v,i}$  is a tight  $(\{2, 4\}, 4)$ -sphere if and only if  $\gcd(v, i) = 1$ . All tight  $(\{2, 4\}, 4)$ -spheres are obtained in

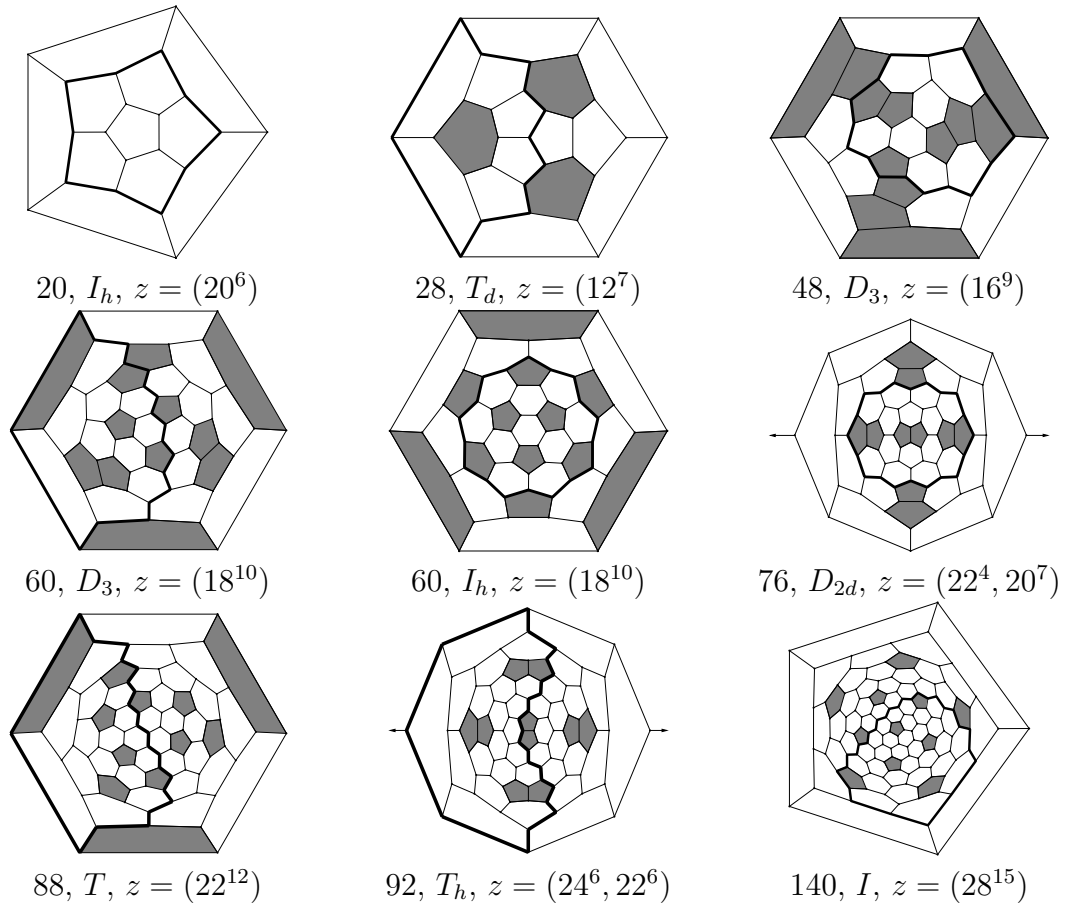


Figure 2.6: All known tight  $(\{5, 6\}, 3)$ -spheres with simple zigzags;  $z$  is the list of lengths of the zigzags

this way. The non-tight  $(\{2, 4\}, 4)$ -spheres are obtained by replacing the central circuits by railroads, which do not self-intersect.

**Remark 2.2.3** *The number of zigzags in a tight  $(\{a, 6\}, 3)$ -sphere is  $\leq 3$ , 3 for  $a = 2, 3$  and, conjecturally  $\leq 8$ ,  $\leq 15$  for  $a = 4, 5$  (see [DeDu05]). The number of central circuits in a tight  $(\{a, 4\}, 4)$ -sphere is 2,  $\leq 6$  for  $a = 2, 3$  (see [DeSt03]). The number of tight  $(\{a, 6\}, 3)$ -spheres with only simple zigzags is 0,  $\infty$ , 2 for  $a = 2, 3, 4$  and, conjecturally, 9 for  $a = 5$  (see Figure 2.6 and [DeDu05]). The number of tight  $(\{a, 4\}, 4)$ -spheres with only simple central circuits is  $\infty$ , 8 for  $a = 2, 3$  (including the right one on Figure 2.4. See [DeSt03, DDS03] for details).*

The polyhedra, which are dual to the 3-valent polyhedra without  $b$ -gonal faces,  $b > 6$ , are studied in [Thu98]; they are called there *non-negatively curved triangulations*. Thurston developed there a global theory of parameter space for sphere triangulations with degree of vertices at most 6. The main Theorem 0.1 there describes them as the elements of  $L_+/G$ , where  $L$  is a lattice in complex Lorenz space  $C^{(1,9)}$ ,  $G$  is a group of automorphisms and  $L_+$  is the set of lattice points of positive square-norm. Clearly, our  $(\{a, 6\}, 3)$ -spheres with  $a = 3, 4, 5$  are covered by Thurston consideration. Let  $s$  denote the number of vertices of degree less than 6; such vertices reflect positive curvature of the triangulation of the sphere  $\mathbb{S}^2$ . Thurston has built a parameter space with  $s - 2$  degrees of

freedom (complex numbers). Using this, Theorem 3.4 in [Sah94] (which is an application of a preliminary version of [Thu98]) implied that the number of  $(\{3, 6\}, 3)$ -,  $(\{4, 6\}, 3)$ -,  $(\{5, 6\}, 3)$ -spheres with  $v$  vertices grows like  $O(v)$ ,  $O(v^3)$ ,  $O(v^9)$ . We believe, that the hypothesis on degree of vertices (in dual terms, that the graph has no  $b$ -gonal faces with  $b > 6$ ) in [Thu98] is unnecessary to his theory of parameter space. Also, his theory can be extended, perhaps, to the case of quadrangulations instead of triangulations.

The graphs, that can be described in terms of Goldberg-Coxeter construction, can be thought as those expressed in terms of one complex parameter. Considering intermediate symmetry groups (for example,  $(\{5, 6\}, 3)$ -polyhedra of symmetry  $D_5$ ), one can use a small number of complex parameters to describe them and this is, actually, done in [Dut02] or in [FCS88] for generating them up to a large number of vertices. For general classes of graphs with no hypothesis on symmetry, the best is, probably, to use CPF ([BDDH97]) or ENU ([Hei98]), which generates all 3- or 4-valent graph with the number of faces of size  $i$  being given in advance.

**Remark 2.2.4** *The possible symmetries of  $(\{2, 3\}, 6)$ -spheres have not been determined yet. Also, the Goldberg-Coxeter construction has not been defined for 6-valent spheres, although we do not see an obstruction to it. Also it could be interesting to extend remark 2.2.3 on those spheres.*

*For the  $(\{2, 3\}, 6)$ -spheres, a useful transformation for computer enumeration and theoretical purposes is the following. Take the dual, which is a plane graph with 6-gonal faces and vertices of degree 2 or 3; then remove the 2-valent vertices. The resulting sphere is a 3-valent one with faces of gonality at most 6. One can so generate a lot of  $(\{2, 3\}, 6)$ -spheres: just take a 3-valent plane graph with faces of size at most 6, put adequately some vertices on some edges and then take the dual.*

We now list the known results on symmetry of those spheres:

**Theorem 2.2.5** *The symmetry groups are as follows:*

- (i) ([GrZa74]) *For  $(\{2, 6\}, 3)$ -spheres, it is one of  $D_3$  or  $D_{3h}$ .*
- (ii) ([FoCr97]) *For  $(\{3, 6\}, 3)$ -spheres, it is one of  $D_2$ ,  $D_{2h}$ ,  $D_{2d}$ ,  $T$ ,  $T_d$ .*
- (iii) ([DeDu05]) *For  $(\{4, 6\}, 3)$ -spheres, it is one of 16 groups:  $C_1$ ,  $C_s$ ,  $C_2$ ,  $C_i$ ,  $C_{2\nu}$ ,  $C_{2h}$ ,  $D_2$ ,  $D_3$ ,  $D_{2d}$ ,  $D_{2h}$ ,  $D_{3d}$ ,  $D_{3h}$ ,  $D_6$ ,  $D_{6h}$ ,  $O$ ,  $O_h$ .*
- (iv) ([FoMa95]) *For  $(\{5, 6\}, 3)$ -spheres, it is one of 28 groups:  $C_1$ ,  $C_2$ ,  $C_i$ ,  $C_s$ ,  $C_3$ ,  $D_2$ ,  $S_4$ ,  $C_{2\nu}$ ,  $C_{2h}$ ,  $D_3$ ,  $S_6$ ,  $C_{3\nu}$ ,  $C_{3h}$ ,  $D_{2h}$ ,  $D_{2d}$ ,  $D_5$ ,  $D_6$ ,  $D_{3h}$ ,  $D_{3d}$ ,  $T$ ,  $D_{5h}$ ,  $D_{5d}$ ,  $D_{6h}$ ,  $D_{6d}$ ,  $T_d$ ,  $T_h$ ,  $I$ ,  $I_h$ .*
- (v) ([DDS03]) *For  $(\{2, 4\}, 4)$ -spheres, it is one of  $D_{4h}$ ,  $D_4$ ,  $D_{2h}$ ,  $D_{2d}$ ,  $D_2$ .*
- (vi) ([DDS03]) *For  $(\{3, 4\}, 4)$ -spheres, it is one of 18 groups:  $C_1$ ,  $C_s$ ,  $C_2$ ,  $C_{2\nu}$ ,  $C_i$ ,  $C_{2h}$ ,  $S_4$ ,  $D_2$ ,  $D_{2d}$ ,  $D_{2h}$ ,  $D_3$ ,  $D_{3d}$ ,  $D_{3h}$ ,  $D_4$ ,  $D_{4d}$ ,  $D_{4h}$ ,  $O$ ,  $O_h$ .*

Another interesting class of spheres, which could be considered, consists of the self-dual ones, whose vertices are of degree 3 or 4 and faces have gonality 3 or 4. The medials (defined in Section 2.1) of such spheres are  $(\{3, 4\}, 4)$ -spheres. In particular,  $p_3 + v_3 = 8$ , which implies  $p_3 = v_3 = 4$ . Furthermore, the self-duality becomes an ordinary symmetry of the  $(\{3, 4\}, 4)$ -sphere.

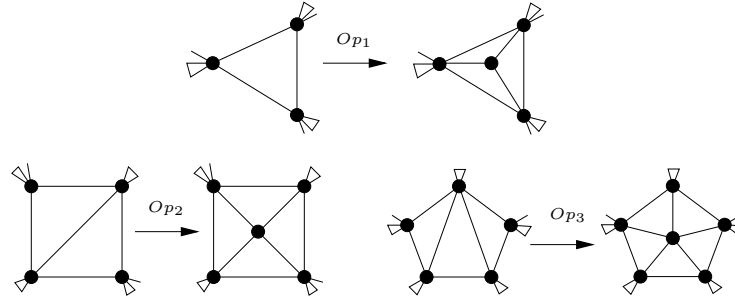
## 2.3 Computer generation of the classes

We now present the general ideas on computer generation of those classes of plane graphs. The main technique in combinatorial construction is the exhaustive search: we build a plane graph, face by face, until it is completed. The main problem is that the number of possibilities to be considered is, usually, very large. Sometimes, one can prove that a group of faces cannot be completed to the desired graph and this yields speedup. But in practice, the benefit, while tremendous, does not change the nature of the problem. Typical examples of this scheme of combinatorial enumeration are presented in Chapters 5 and 10.

The main and fundamental objection is that one needs, sometimes, to make huge computations lasting months for finding only a few graphs. Fortunately, for above classes, there are some other ways to diminish the magnitude of the problem. A simple zigzag or central circuit (see Figure 2.4 for some examples) splits the sphere into two parts, which are much easier to enumerate. Of course, all is not so easy in practice since a zigzag or central circuit is self-intersecting most of the time. But the basic idea remains (see [BHH03]) and is used in the following programs:

1. The program **CPF** ([BDDH97]) generates 3-valent plane graphs with specified  $p$ -vector.
2. The program **ENU** ([BHH03] and [Hei98]) does the same for 4-valent plane graphs.
3. The program **CGF** ([Har]) generates 3-valent orientable maps with specified genus and  $p$ -vector.

If one considers a larger class, like the plane triangulations, then another strategy is possible. It is known (see [Ebe1891]) that every plane triangulation arises from Tetrahedron by a sequence of three following operations  $Op_i$ :



Of course, there is a very large number of triangulations. But the running time of the algorithm is approximately proportional to the number of triangulations to be found and it scales with almost 100% efficiency on parallel computers. Note also that the above algorithm is not limited by memory: for a given plane triangulations  $T$ , there are many ways of using the operations  $Op_i$  to obtain  $T$  from Tetrahedron. But the canonical augmentation scheme (see [McK98]) provides a unique application of the  $Op_i$ , in order to get  $T$ , thereby avoiding memory problems.

The enumeration of triangulations, triangulations of minimum degree 4 or 5, Eulerian triangulations, quadrangulations, 3-connected plane graphs, plane graphs, 3-connected plane graphs of minimum degree at least 4 or 5 is done in the program **plantri** (see [BrMK], [BrMK06] and [BGGMTW05]) using such kind of elementary operations. There

is no reasonable hope of applying this kind of algorithm to the enumeration of  $(\{a, b\}, k)$ -spheres because there is no simple operation like the  $Op_i$  that would preserve the property of being a  $(\{a, b\}, k)$ -sphere.

All computations used the **GAP** computer algebra system [GAP] and the package Plan-Graph ([Dut02]) by the second author; the programs are available from [Du07].

The program **CaGe** ([BDDH97]) was used for most of the graph drawings.

# Chapter 3

## Fullerenes as tilings of surfaces

The discovery of the fullerene molecules and related forms of carbon, such as nanotubes, has generated an explosion of activity in Chemistry, Physics and Materials Science, which is amply documented, for example, in [DDE96] and [FoMa95]. In Chemistry, the “classical” definition is that a fullerene is an all-carbon molecule in which the atoms are arranged as a map on sphere made up entirely of 5-gons and 6-gons, which therefore, necessarily includes exactly 12 5-gonal faces. We are concerned here with a generalization in the following direction: what fullerenes are possible if a fullerene is a finite 3-valent map with only 5- and 6-gonal faces embedded in any surface? This seemingly much larger concept leads only to three extensions to the class of spherical fullerenes. Embedding in only four surfaces is possible (see [DFRR00] for details): the sphere, torus, Klein bottle and projective plane. The usual spherical fullerenes have 12 5-gons, projective fullerenes 6, and toric and Klein bottle fullerenes none. Klein bottle and projective fullerenes are the antipodal quotients of centrally symmetric toric and spherical fullerenes, respectively. Extensions to infinite graphs (plane fullerenes, cylindrical fullerenes) are indicated. Detailed treatment of the concept of the extended fullerenes and their further generalization to higher dimensional manifolds is given in [DeSt99b].

### 3.1 Classification of finite fullerenes

Define a *3-fullerene* as a 3-valent map embedded on a surface and consisting of only 5-gonal and 6-gonal faces. Each such object has, say,  $v$  vertices,  $e$  edges and  $f$  faces of which  $p_5$  are 5-gons and  $p_6$  are 6-gons.

From Theorem 1.2.3, we know that the Euler characteristic  $\chi$  satisfies to

$$p_5 = 6\chi,$$

For a surface, in which a finite 3-fullerene can be embedded, the number  $\chi$  is, therefore, a non-negative integer. Let us use the classification of compact surfaces in Theorem 1.2.1 and recall the expression of  $\chi$  in Theorem 1.2.2:

$$\begin{aligned}\chi &= 2(1 - g) && \text{(for an orientable surface)} \\ &= 2 - g && \text{(for a non-orientable surface).}\end{aligned}$$

The cases compatible with non-negative integral solutions for  $\chi$  are thus exactly four in number. The only surfaces admitting finite 3-fullerene maps are therefore:  $\mathbb{S}^2$  (the sphere,

orientable with  $g = 0$ ),  $\mathbb{T}^2$  (the torus, orientable with  $g = 1$ ),  $\mathbb{P}^2$  (the projective plane, non-orientable with  $g = 1$ ) and  $\mathbb{K}^2$  (the Klein bottle, non-orientable with  $g = 2$ ). All embeddings are *2-cell-embeddings*, i.e., each face is homeomorphic to an open disk. An immediate consequence of Euler formula is that fullerenes on  $\mathbb{S}^2$ ,  $\mathbb{T}^2$ ,  $\mathbb{K}^2$  and  $\mathbb{P}^2$  have exactly 12, 0, 0 and 6 5-gons, respectively. Toric and Klein bottle fullerenes may also be called toric and Klein bottle *polyhexes* ([FYO95, Kir94, Kir97, KlZh97]) as they include no 5-gons.

Figure 3.1 shows smallest fullerenes from the four classes, drawn as the graph, the map and its dual triangulation in the appropriate surface. Remark that the Petersen and Heawood graphs which appear naturally here are, actually, the 5- and 6-cages (a  $k$ -cage is a 3-valent graph of smallest cycle size  $k$  with the largest possible number of edges); their duals in  $\mathbb{P}^2$  and  $\mathbb{T}^2$ ,  $K_6$  and  $K_7$ , realize the *chromatic number* (i.e., minimal number of colors, which a map on surface can be with colored, so that no two faces of same color are adjacent; see, for example, [GrTu87, Chapter 5]) of the corresponding surfaces.

Spherical and toric fullerenes have an extensive chemical literature, and Klein bottle polyhexes have been considered, for example, in [Kir97, KlZh97].

Remind that at least one spherical fullerene with  $v$  vertices exists for all even  $v$  with  $v \geq 20$ , except for the case  $v = 22$  ([GrMo63]).

## 3.2 Toric and Klein bottle fullerenes

$(6, 3)$ -tori and  $(6, 3)$ -Klein bottles are related to  $\{6, 3\}$  in a straightforward way. The underlying surfaces are quotients of the Euclidean plane  $\mathbb{R}^2$  under groups of isometries generated by two translations (for  $\mathbb{T}^2$ ) or one translation and one glide reflection (for  $\mathbb{K}^2$ ). Each point of  $\mathbb{T}^2$  and  $\mathbb{K}^2$  corresponds to an orbit of the generating group. Note that the groups generated by a single translation or a single reflection, respectively, give, as quotients, the cylinder and the twisted cylinder (the Möbius strip, see Figure 1.1). Construction and enumeration of polyhexes can therefore be envisaged as a process of cutting parallelograms out of the “graphite plane”  $\{6, 3\}$  and gluing their edges according to the rules implied in Figure 3.1.

Some confusion exists in the mathematical and chemical literature on toric polyhexes. Negami ([Neg85]), Altschuler ([Alt73]) and other topological graph theorists define regular 3-valent maps on the torus to mean 2-cell embeddings with all faces 6-gonal, without further qualification. Coxeter and others, working in a group theoretical tradition, use the same term in a more restricted sense of polyhexes with automorphism groups  $Aut(G)$  of the maximal possible order, in other words, those that realize the equality in the bound  $|Aut(G)| \leq 4e(G)$  ( $= 6p_6$  for a polyhex). All such regular maps are: (on  $\mathbb{S}^2$ ) the five Platonic polyhedra, (on  $\mathbb{P}^2$ ) six graphs that include the Petersen graph and its dual, (on  $\mathbb{K}^2$ ) no graphs at all ([Nak96]), and (on  $\mathbb{T}^2$ ) the polyhexes that arise by the Goldberg-Coxeter construction from the 6-gon (see Section 2.1).

In Negami’s construction ([Neg85]), a three-parameter code represents any toric polyhex (or, equivalently, any 6-regular triangulation of  $\mathbb{T}^2$ ) as a tiling of  $\{6, 3\}$ . Each graph of this type is denoted  $T(p, q, r)$ , with integer parameters  $p$ ,  $q$  and  $r$  where  $p$  is the length of a geodesic cycle of edge-sharing 6-gons,  $r$  is the number of such cycles and  $q$  is an offset.

At least one toric polyhex, which is cell-complex exists for all numbers of vertices  $v \geq 14$ . The unique cell-complex toric fullerene at  $v = 14$  is a realization of the Heawood graph. It is  $GC_{2,1}(\text{hexagon})$  in terms of Goldberg-Coxeter construction and is the dual of

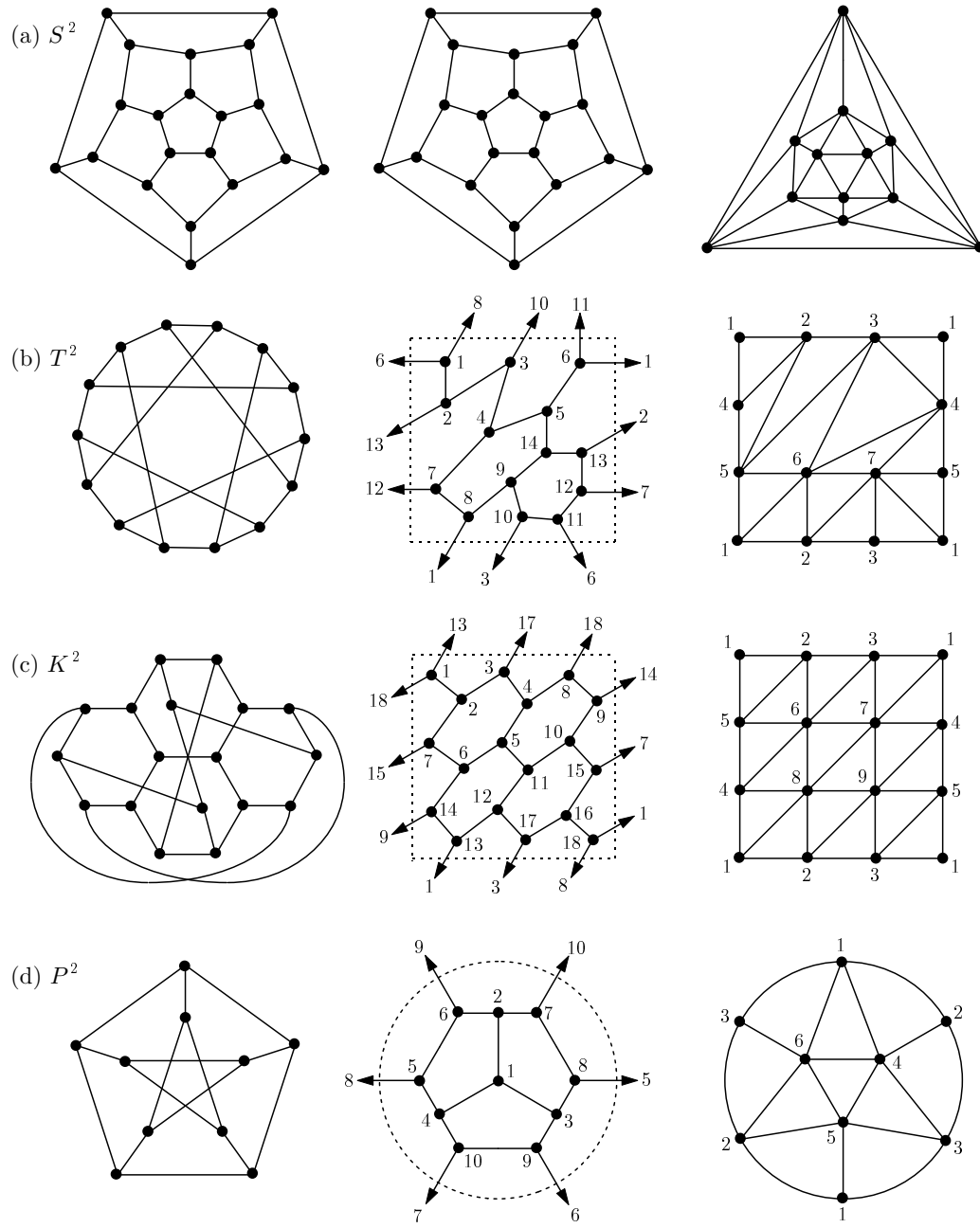


Figure 3.1: Smallest spherical, toric, Klein bottle and projective fullerenes. The first column lists the graphs drawn in the plane, the second the map in the appropriate surface and the third the dual in the same surface. The examples are: (a) Dodecahedron (dual Icosahedron), (b) the Heawood graph (dual  $K_7$ ), (c) a smallest Klein bottle polyhex (dual  $K_{3,3,3}$ ) and (d) the Petersen graph (dual  $K_6$ ).

$K_7$ , which itself realizes the 7-color map on the torus. This map and its dual are shown in Figure 3.1.

A description of Klein bottle polyhexes can be developed along similar lines ([Nak96]). Each toric graph  $T(p, 0, r)$  can be used to obtain two Klein bottle 6-regular triangulations (and hence, by taking dual, 3-fullerenes), the *handle* and *cross-cap* types  $K_h(p, r)$  and  $K_c(p, r)$ , respectively. The torus is cut along a geodesic of length  $p$ . Then the *handle* construction amounts to identification of opposite sides of the resulting parallelogram with reversed direction. In the *cross-cap* construction, the opposite sides are each converted to cross-caps, with slightly different rules for odd and even  $p$ . The unique smallest cell-complex Klein bottle polyhex has 18 vertices (9 6-gonal faces) and is the dual of the tripartite  $K_{3,3,3}$ ; the graph, the map and its dual are shown in Figure 3.1.

### 3.3 Projective fullerenes

The projective plane arises as a quotient space of the sphere, the required group being  $C_i$ . It is obtained by identifying antipodal points of the spherical surface; in other words, it is the antipodal quotient of the sphere (see Section 1.2.2).  $\mathbb{P}^2$  is the simplest compact non-orientable surface in the sense that it can be obtained from the sphere by adding just one cross-cap.

Clearly, this construction can be carried over to maps: the antipodal quotient of a centrosymmetric map on the sphere has vertices, edges and faces obtained by identifying antipodal vertices, edges and faces, thereby halving the number of each type of structural component. For example, the antipodal quotient of Icosahedron is  $K_6$ , and that of Dodecahedron is the Petersen graph, famous as a counterexample to many conjectures (see, for example, [HoSh93]). The Petersen graph is not a planar graph but it is called *projective-planar* in the sense that it can be embedded without edge crossings in the projective plane.

In this terminology, our definition of projective fullerenes amounts to selection of cell-complex projective-planar 3-valent maps with only 5- and 6-gonal faces. As noted above,  $p_5 = 6$  for these maps. Thus, the Petersen graph is the smallest projective fullerene. In general, the projective fullerenes are exactly the antipodal quotients of the centrally symmetric spherical fullerenes.

Thus, the problem of enumeration and construction of projective fullerenes reduces simply to that for centrally symmetric conventional spherical fullerenes. The point symmetry groups that contain the inversion operation are  $C_i$ ,  $C_{mh}$ , ( $m$  even),  $D_{mh}$  ( $m$  even),  $D_{md}$  ( $m$  odd),  $T_h$ ,  $O_h$  and  $I_h$ . A spherical fullerene may belong to one of 28 point groups ([FoMa95]) of which 8 appear in the previous list:  $C_i$ ,  $C_{2h}$ ,  $D_{2h}$ ,  $D_{6h}$ ,  $D_{3d}$ ,  $D_{5d}$ ,  $T_h$  and  $I_h$ . Clearly, a fullerene with  $v$  vertices can be centrally symmetric only if  $v$  is divisible by four as  $p_6$  must be even. After the minimal case  $v = 20$ , the first centrally symmetric fullerenes are at  $v = 32$  ( $D_{3d}$ ) and  $v = 36$  ( $D_{6h}$ ).

### 3.4 Plane 3-fullerenes

An example of infinite 3-fullerene is given by *plane fullerenes*, i.e., 3-valent partitions of the plane into (combinatorial) 6-gons and  $p_5$  5-gons. Such partitions have  $p_5 \leq 6$  (see [DeSt02b] for a reduction of proof to Alexandrov theory in [Ale50] and [Ale48, Chapter

VIII)]. For  $p_5 = 0, 1$  such 3-fullerene is unique; for any  $2 \leq p_5 \leq 6$  there is an infinity of them.



# Chapter 4

## Polycycles

### 4.1 $(r, q)$ -polycycles

A  $(r, q)$ -*polycycle* is a simple plane 2-connected locally finite graph with degree at most  $q$ , such that it holds:

- (i) all interior vertices are of degree  $q$ ,
- (ii) all interior faces are (combinatorial)  $r$ -gons.

Remind that any finite plane graph has a unique exterior face; an infinite plane graph can have any number of exterior faces, including zero and infinity. Denote by  $p_r$  the number of interior faces; for example, Dodecahedron on the plane has  $p_5 = 11$ .

See on Figure 4.1 some examples of connected simple plane graphs, which are not  $(r, q)$ -polycycles.

We will prove later (in Theorem 4.3.2) that all vertices, edges and interior faces of a  $(r, q)$ -polycycle form a cell-complex (see Section 1.2.1).

The *skeleton of a polycycle* is the edge-vertex graph defined by it, i.e., we forget the faces. By Theorem 4.3.6, except for five Platonic ones, the skeleton has a unique *polycyclic realization*, i.e., a polycycle for which it is the skeleton.

The parameters  $(r, q)$  are called *elliptic* if  $rq < 2(r + q)$ , *parabolic* if  $rq = 2(r + q)$ , and *hyperbolic* if  $rq > 2(r + q)$ ; see Remark 1.4.1. Call a polycycle *outerplanar* if it has no interior vertices. For parabolic or hyperbolic  $(r, q)$ , the tiling  $\{r, q\}$  is a  $(r, q)$ -polycycle. For elliptic  $(r, q)$ , the tiling  $\{r, q\}$  with a face deleted is a  $(r, q)$ -polycycle. Different, but all isomorphic, polycyclic realizations for those five exceptions to the unicity, come from different choices of such deleted (exterior) face.

The  $(r, q)$ -polycycles  $\{r, q\}$  with parabolic and hyperbolic parameters  $(r, q)$  do not have a boundary.

Recall that an *isomorphism* between two plane graphs,  $G_1$  and  $G_2$ , is a function  $\phi$  mapping vertices, edges and faces of  $G_1$  to the ones of  $G_2$  and preserving incidence

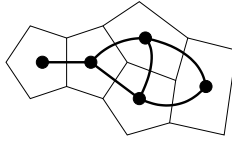


Figure 4.1: Some plane graphs, which are not  $(r, q)$ -polycycles

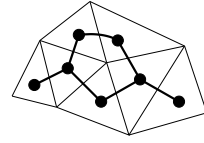
relations. Two  $(r, q)$ -polycycles,  $P_1$  and  $P_2$ , are *isomorphic* if there is an isomorphism  $\phi$  of their skeletons preserving the set of interior faces. Recall also that the *automorphism group*  $Aut(G)$  of a plane graph  $G$  is the group of all its *automorphisms*, i.e., isomorphisms of  $G$  to  $G$ . The *automorphism group*  $Aut(P)$  of a polycycle  $P$  consists of all automorphisms of plane graph  $G$  preserving the set of interior faces.

The notion of duality of plane graphs applies as well for  $(r, q)$ -polycycles, but it ignores the exterior faces, which we want to keep unchanged. We will introduce two notions of duality for  $(r, q)$ -polycycles and call them *inner dual* (see [BCH02] for some applications in enumeration) and *outer dual*. They are always defined, but the resulting plane graph is not necessarily a  $(q, r)$ -polycycle.

The inner dual  $Inn^*(P)$  of an  $(r, q)$ -polycycle  $P$  is the graph obtained by taking the interior faces as vertices and having, as edges, the edges between two adjacent interior faces. The inner dual  $Inn^*(P)$  is not necessarily 2-connected. See below two examples:

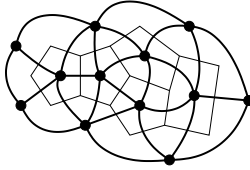


A  $(5, 3)$ -polycycle and its inner dual

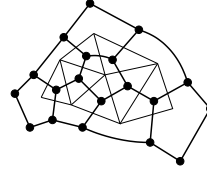


A  $(3, 5)$ -polycycle and its inner dual

The outer dual  $Out^*(P)$  of an  $(r, q)$ -polycycle  $P$  is the graph obtained by taking, as vertex-set, the interior faces and some exterior vertices. Such exterior vertices are taken around every boundary vertex of  $P$ , so as to make sure that they correspond to  $q$ -gonal faces of  $Out^*(P)$ . The degree of boundary vertices may be higher than  $r$ . Another possible obstruction to  $Out^*(P)$  being a  $(q, r)$ -polycycle is not having any exterior face, as can happen for the tiling  $\{r, q\} - f$  with elliptic  $(r, q)$ . See below two examples:



A  $(5, 3)$ -polycycle and its outer dual



A  $(3, 5)$ -polycycle and its outer dual

One has the equality  $P = Inn^*(Out^*(P))$  and  $P = Out^*(Inn^*(P))$  for an  $(r, q)$ -polycycle  $P$ , provided that all the maps appearing in those equations are  $(r, q)$ - or  $(q, r)$ -polycycles. If all operations are defined correctly and  $P$  is an  $(r, q)$ -polycycle, then  $Inn^*(Inn^*(P))$  is the  $(r, q)$ -polycycle  $P$  with all  $r$ -gons having boundary edges removed, while  $Out^*(Out^*(P))$  is the  $(r, q)$ -polycycle  $P$  with a ring of  $r$ -gons being added on its outermost layer, so that all boundary vertices become interior vertices.

Call a polycycle *proper* if it is a partial subgraph of  $\{r, q\}$  and a *helicene*, otherwise (this term will be justified later by Theorem 4.3.1). Call a proper  $(r, q)$ -polycycle *induced* (moreover, *isometric*) if this subgraph is, in addition, induced (moreover, isometric) subgraph of  $\{r, q\}$ . Other interesting possible property of a proper  $(r, q)$ -polycycle is being convex in  $\{r, q\}$  (see Theorem 4.4.1).

For  $(r, q) = (3, 3), (4, 3), (3, 4)$ , any induced  $(r, q)$ -polycycle is isometric but, for example, the path of three 5-gons is induced non-isometric  $(5, 3)$ -polycycle.

Consider now the notion of reciprocity, defined for some proper polycycles. Let  $P$  be a proper bounded  $(r, q)$ -polycycle. Consider the union of all  $r$ -gonal faces of  $\{r, q\}$

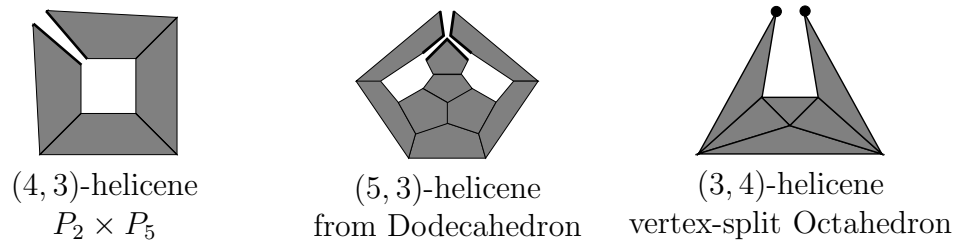


Figure 4.2: Some small helicenes

outside of  $P$ . Easy to see that this union will be an  $(r, q)$ -polycycle; call it then *reciprocal polycycle* to  $P$  if either  $P$  is elliptic, or  $P$  is infinite and has connected boundary. Call a polycycle *self-reciprocal* if it admits the reciprocal polycycle and is isomorphic to it.

All self-reciprocal  $(r, q)$ -polycycles with  $(r, q) = (3, 3), (4, 3), (3, 4), (5, 3)$  are:  $\{3, 3\} - e$ ,  $\{4, 3\} - v$ ,  $P_2 \times P_4$ ,  $\{3, 4\} - v$ ,  $\{3, 4\} - C_3$ ,  $Tr_4$  and 9 (out of 11)  $(5, 3)$ -polycycles with  $p_5 = 6$ , including 6 chiral ones. An example of self-reciprocal  $(3, q)$ -polycycle, for any  $q \geq 3$ , is a  $(3, q)$ -polycycle on one of two shores of *zigzag* (see definition in Section 2.2), cutting  $\{3, q\}$  in two isomorphic halves; it includes  $\{3, 3\} - e$ ,  $\{3, 4\} - C_3$  and is infinite for  $q \geq 6$ .

A general theory of polycycles is considered in [DeSt98, DeSt99a, DeSt02c, DeSt00a, DeSt00b, DeSt00c, DeSt01, DeSt02b, Sht99, Sht00].

## 4.2 Examples

Call an  $(r, q)$ -polycycle *elliptic*, *parabolic* or *hyperbolic*, if  $rq < 2(r + q)$ ,  $rq = 2(r + q)$  or  $rq > 2(r + q)$ . This corresponds to  $\{r, q\}$  being the regular tiling of  $S^2$ ,  $\mathbb{R}^2$  or  $\mathbb{H}^2$ , respectively.

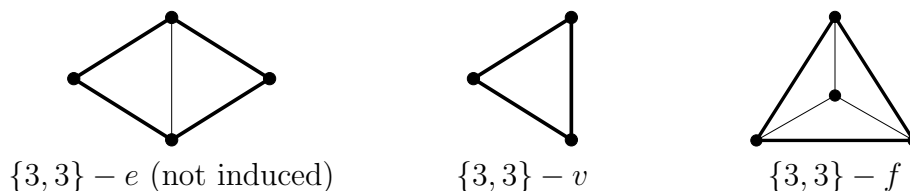
There is a literature (see, for example, [GrSh87a, Section 9.4], [BGOR99], [BCH02] and [BCH03]) about proper parabolic polycycles (*polyhexes*, *polyamonds*, *polyominoes* for  $\{6, 3\}$ ,  $\{3, 6\}$ ,  $\{4, 4\}$ , respectively); the terms come from familiar terms *hexagon*, *diamond*, *domino*, where the last two correspond to the case  $p_3, p_4 = 2$ .

Polyominoes were considered first by Conway, Penrose, Colomb as tiles (of  $\mathbb{R}^2$  etc.; see, for example, [CoLa90]) and in Game Theory; later, they were used for enumeration in Physics and Statistical Mechanics.

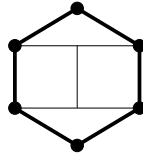
Polyhexes are used widely (see, for example, [Dia88, Bal95]) in Organic Chemistry: they represent *completely condensed PAH* (*polycyclic aromatic hydrocarbons*)  $C_nH_m$  with  $n$  vertices (atoms of the carbon C), including  $m$  vertices of degree two, where atoms of the hydrogen  $H$  are adjoined (see Figure 7.1).

All 39 proper  $(5, 3)$ -polycycles were found in [CCBBZGT93] in chemical context, but already in [Har90] were given all 3, 6, 9, 39, 263 proper elliptic  $(r, q)$ -polycycles for  $(r, q) = (3, 3), (4, 3), (3, 4), (5, 3), (3, 5)$ , respectively.

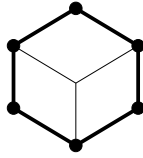
Now, we list all  $(3, 3)$ -,  $(4, 3)$ -,  $(3, 4)$ -polycycles. Clearly, all  $(3, 3)$ -polycycles are:



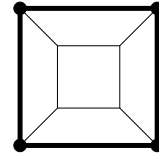
Recall that  $P_n$  denotes a path with  $n$  vertices; denote by  $P_{\mathbb{N}}, P_{\mathbb{Z}}$  infinite paths in one or both directions. All  $\{4, 3\}$ -polycycles are:



$\{4, 3\} - e$

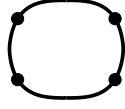


$\{4, 3\} - v$

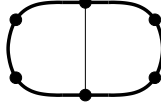


$\{4, 3\} - f$

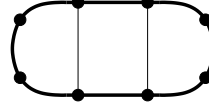
the infinite series  $P_2 \times P_n$  (for any  $n \geq 2$ ; see below examples with  $n = 2, 3, 4$ ):



$P_2 \times P_2$

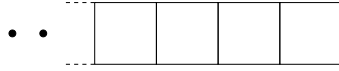


$P_2 \times P_3$

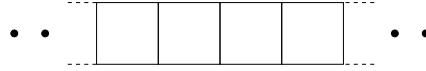


$P_2 \times P_4$

and two infinite ones:



$P_2 \times P_{\mathbb{N}}$

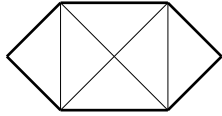


$P_2 \times P_{\mathbb{Z}} = Prism_{\infty}$

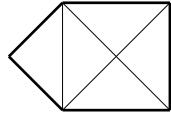
Only  $\{4, 3\}$ ,  $\{4, 3\} - v$ ,  $P_2 \times P_2$ ,  $P_2 \times P_3$ ,  $P_2 \times P_4$ ,  $\{4, 3\} - e$  are proper; amongst them only the last two are not induced.

The number of  $\{3, 4\}$ -polycycles is also countable, including two infinite ones (9 of  $\{3, 4\}$ -polycycles are proper and 5 of proper ones are induced).

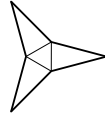
Namely, all  $\{3, 4\}$ -polycycles are:



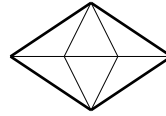
vertex-split  $\{3, 4\}$



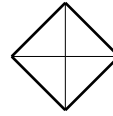
$\{3, 4\} - P_3$



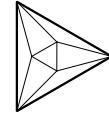
$\{3, 4\} - C_3$



$\{3, 4\} - e$



$\{3, 4\} - v$

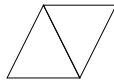


$\{3, 4\} - f$

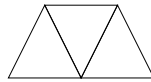
the infinite series  $Tr_n$  (for any  $n \geq 1$ ; see below examples with  $n = 1, 2, 3, 4$ ):



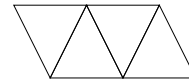
$Tr_1$



$Tr_2$

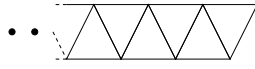


$Tr_3$

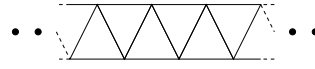


$Tr_4 = \{3, 4\} - P_4$

and two infinite ones:



$Tr_{\mathbb{N}}$



$Tr_{\mathbb{Z}} = APrism_{\infty}$

For all other parameters  $(r, q)$ , there is a continuum of  $(r, q)$ -polycycles and the number of finite ones amongst them is countable.

The *vertex-split Octahedron* and the *vertex-split Icosahedron* are polycycles obtained from Octahedron and Icosahedron, respectively, by splitting a vertex into two vertices and the edges, incident to it, in two parts, accordingly. The vertex-split Octahedron is drawn on Figure 4.2<sup>1</sup>, and both of them are given on Figure 8.3; they are only, besides five Platonic  $\{r, q\} - f$ , non-extensible finite  $(r, q)$ -polycycles.

<sup>1</sup>It is the *Hexagon*, HSBC logo from 1983; it was developed from bank's 19<sup>th</sup> century house flag: white rectangle divided diagonally to produce a red hourglass shape. This flag was derived from Scottish flag: *saltire* or *crux decussata* (heraldic symbol in the form of diagonal cross); Saint Andrew was crucified upon and 13<sup>th</sup> century tradition states that the cross was X-shaped at his own request, out of respect for Jesus.

### 4.3 Cell-homomorphism and structure of $(r, q)$ -polycycles

Given two maps  $X$  and  $X'$ , recall that a *cell-homomorphism* is a function  $\phi : X \rightarrow X'$  that transforms vertices, edges, faces of  $X$  to vertices, edges, faces of  $X'$  while preserving the incidence relations. Recall also that a *flag*  $h$  of a map  $X$  is a sequence  $h = (v, e, f)$  with  $v, e, f$  being a vertex, edge, face of  $X$  and  $v \in e \subset f$ . For a flag  $h = (v, e, f)$  of a polycycle  $P$ ,  $f$  is necessarily an interior face.

**Theorem 4.3.1** ([DeSt98, GHZ02, Gra03]) *Any  $(r, q)$ -polycycle  $P$  admits a cell-homomorphism into  $\{r, q\}$  and such homomorphism is defined uniquely by a flag and its image.*

**Proof.** Given a flag  $h = (v, e, f)$  of  $P$ , recall that  $\sigma_0(h)$ ,  $\sigma_1(h)$  and  $\sigma_2(h)$  (see Section 1.2.2) are unique flags, if they exist, differing from  $h$  on  $v$ ,  $e$  and  $f$ , respectively. Given a vertex  $v$  and an edge  $e$  with  $v \in e$ , there exists at least one face  $f$  of  $P$  such that  $(v, e, f)$  is a flag.

Given a vertex  $v$ , consider the set  $\mathcal{F}_v$  of flags  $(v, e, f)$ . If  $v$  is an interior vertex, then, clearly, any two flags  $h, h' \in \mathcal{F}_v$  are related by a sequence of operations  $\sigma_1$ , and  $\sigma_2$ . If  $v$  belongs to the boundary, then, since  $v$  cannot disconnect the graph, the vertex corona of  $v$  contains only one exterior face. This means that, again, any two flags  $h, h'$  in  $\mathcal{F}_v$  are related by operations  $\sigma_1$  and  $\sigma_2$ . Since the graph, underlying the polycycle, is connected, any two flags are related by a sequence of operations  $\sigma_0$ ,  $\sigma_1$  and  $\sigma_2$ .

Given a cell-homomorphism  $\phi$ , the operations on flags should satisfy to  $\phi(\sigma_i(h)) = \sigma_i(\phi(h))$  for any  $i = 0, 1, 2$ . Consider a flag  $h_0$  in  $P$  and  $k_0$  in  $\{r, q\}$ . Any other flag  $h$  in  $P$  is related to  $h_0$  by a sequence of operations  $\sigma_i$ . Hence, if  $\phi(h_0) = k_0$ , then  $\phi(h)$  is completely determined. This proves the uniqueness of  $\phi$ . But this also give a way to prove the existence of an homomorphism  $\phi$  with  $\phi(h_0) = h'_0$ . In fact, define  $\phi(h) = \sigma_{i_1} \dots \sigma_{i_t}(k_0)$  with  $h = \sigma_{i_1} \dots \sigma_{i_t}(h_0)$  and  $0 \leq i_j \leq 2$ . Since tiling  $\{r, q\}$  has no boundary, all faces are interior and the operations  $\sigma_i$  are always defined in  $\{r, q\}$ .

But, in order for this construction to work, one should prove that  $\phi(h)$  is independent of the expression  $\sigma_{i_1} \dots \sigma_{i_t}$  chosen to express  $h$  in terms of  $h_0$ . Consider two expressions of  $h$ :

$$h = \sigma_{i_1} \dots \sigma_{i_t}(h_0) = \sigma_{i'_1} \dots \sigma_{i'_t}(h_0).$$

Associate to it the flag paths:

$$\begin{aligned} P'' &= (h_0, h_1, \dots, h_t = h) & \text{with} & & h_j &= \sigma_{i_j}(h_{j-1}), \\ P' &= (h'_0 = h_0, h'_1, \dots, h'_t = h) & \text{with} & & h_j &= \sigma_{i'_j}(h'_{j-1}). \end{aligned}$$

Those sequences correspond to vertex sequences, i.e., a path in the  $(r, q)$ -polycycle  $P$ . Locally, there is no obstruction to the coherence of the definition of  $\phi(h)$ . Around a boundary vertex, there is no problem and, around an interior vertex, the condition of having degree  $q$  provides coherence. Also, if one consider flags around a face  $f$ , one does not encounter coherence problems. The simple connectedness of  $P$  allows us to modify the path  $P''$  into the path  $P'$  by changing around face and vertices. So, no ambiguity will appear.  $\square$

All properties, defining  $(r, q)$ -polycycles, were used in the proof of Theorem 4.3.1. In particular, a  $(r, q)$ -polycycles have to be simply connected; see some examples on Figure 4.4.

Clearly, the above cell-homomorphism is an isomorphism if and only if  $P$  is a proper polycycle, i.e., there is no pair of vertices or edges having the same image. In view of Theorem 4.3.1, any improper  $(r, q)$ -polycycle is called  $(r, q)$ -*helicene* (see Figure 4.2). It is easy to check that an  $(r, q)$ -helicene exists if and only if  $(r, q) \neq (3, 3)$  and  $p_r \geq (q - 2)(r - 1) + 1$  with equality only for the helicene being a ring of  $r$ -gons, going around an  $r$ -gon.

A natural parameter to measure an  $(r, q)$ -helicene, will be the degree of the corresponding homomorphism into  $\{r, q\}$  (on vertices, edges and faces). For  $q \geq 4$ , helicenes appear with vertices, but not edges, having same homomorphic image. The vertex-split Octahedron is unique such maximal helicene for  $(r, q) = (3, 4)$  (two 2-valent vertices are such; see Figure 4.2). There is a finite number of such helicenes for  $(r, q) = (3, 5)$ ; one of them is the vertex-split Icosahedron.

**Theorem 4.3.2** ([DeSt05]) *The vertices, edges and interior faces of any  $(r, q)$ -polycycle form a cell-complex.*

**Proof.** To prove that it is a cell-complex, we shall prove that the intersection of any two cells (i.e., vertices, edges or interior faces) of an  $(r, q)$ -polycycle  $P$  is again a cell of  $P$  or  $\emptyset$ . For intersection of vertices with edges or faces this is trivial. For intersection of edges or faces, we will use the cell-homomorphism  $\phi$  from  $P$  to  $\{r, q\}$ .

If two interior faces  $F$  and  $F'$  of  $P$  intersect in several cells (for example, two edges or two vertices), then their images in  $\{r, q\}$  also intersect in several cells. It is easy to see that this cannot occur in  $\{r, q\}$ . So,  $F$  and  $F'$  intersect in an edge, vertex or  $\emptyset$ . The same proof works for other intersections of cells.  $\square$

**Theorem 4.3.3** *If a finite  $(r, q)$ -polycycle has a boundary vertex whose degree is less than  $q$ , then the total number of these vertices is at least two.*

**Proof.** Take a flag  $f$  in this  $(r, q)$ -polycycle  $P$  and a flag  $f'$  in  $\{r, q\}$ . Let us now use the cell-homomorphism  $\phi$  as in Theorem 4.3.1. The boundary  $\mathcal{B}$  of  $P$  consists of vertices  $v_1, \dots, v_k$ . The image of this boundary in  $\{r, q\}$  is also a cycle  $\phi(\mathcal{B})$ . Whenever  $\mathcal{B}$  has a vertex  $v_i$  of degree  $q$ , the edges  $e_i = v_{i-1}v_i$  and  $e_{i+1} = v_iv_{i+1}$  belong to a common face  $F$ . Assume now, in order to reach a contradiction, that we have only one vertex of degree different from  $q$ . This implies that all  $e_i$  are incident to the same face  $F$ . In particular, the length of the boundary is a multiple of  $r$ . But if one makes turn around a face  $F$ , it must always be on the same direction, i.e., rightmost turn or leftmost turn. So, a vertex of degree different from  $q$  is impossible.  $\square$

The *girth* of a graph is the length of a minimal edge circuit in it.

**Theorem 4.3.4** *For the skeleton of  $\{r, q\}$ , it holds:*

- (i) *its girth is  $r$ ,*
- (ii) *its minimal edge circuits are the boundaries of faces of  $\{r, q\}$ .*

**Proof.** This statement can be easily verified for elliptic  $(r, q)$ . Two edges of Tetrahedron always belong to the same triangle. Two adjacent edges of the same face of Octahedron (or Icosahedron) enter the boundary triangle of the face, while if they do not belong to the same face, then they enter an edge circuit of length at least four. Three successive edges of Cube (or Dodecahedron), belonging to the same face, enter the boundary quadrangle

(pentagon) of the face, while if they do not belong to the same face, then they enter an edge circuit of length at least six.

The verification in the parabolic or hyperbolic case proceeds as follows. Take a simple edge circuit in the tiling  $\{r, q\}$ . By Jordan theorem, this circuit bounds a finite domain in the plane; this domain contains at least one 2-dimensional  $r$ -gon of  $\{r, q\}$ . Draw the rays from the center of this circuit through its vertices. These rays divide the central angle into  $r$  sectors, each sector based on its own side of the  $r$ -gon. Any line connecting two external points of the boundary rays of a sector, is longer than the side of the  $r$ -gon. Therefore, the number of edges in any edge circuit containing the  $r$ -gon and not coinciding with it, is greater than  $r$ . Hence, the girth of the skeleton of the tiling is  $r$ . The assertion (ii) follows in the same way.  $\square$

**Corollary 4.3.5** *For any  $(r, q)$ -polycycle  $P$  it holds:*

- (i)  *$P$  has girth  $r$ , and the length of its boundaries is at least  $r$ .*
- (ii) *If a boundary of  $P$  has length  $r$ , then either  $P$  is an  $r$ -gon, or  $(r, q)$  is elliptic and  $P$  is  $\{r, q\} - f$ .*

**Proof.** The assertion (i) is trivial using Theorem 4.3.4 and 4.3.1. Let us now prove (ii). If the length of a boundary of  $P$  is  $r$ , then  $P$  has only one boundary of finite length and so,  $P$  is a finite polycycle. Let us consider the mapping  $\phi$  from  $P$  to  $\{r, q\}$ . The image of the boundary of  $P$  is a face of  $\{r, q\}$ . If the image lies inside of this  $r$ -gon, then  $P$  is an  $r$ -gon. Otherwise, all boundary vertices of  $P$  have degree  $q$ . Since all vertices of the image of  $P$  in  $\{r, q\}$  have degree  $q$  in  $\{r, q\}$ , one obtains that  $\phi(P)$  covers completely  $\{r, q\}$  except one face. So, the parameters  $(r, q)$  are elliptic and  $P = \{r, q\} - f$ .  $\square$

**Theorem 4.3.6** *Given a graph  $G$ , which is the skeleton of a  $(r, q)$ -polycycle different from (one of 5) elliptic  $\{r, q\}$ , then the polycyclic realization is completely determined by  $G$ .*

**Proof.** From Corollary 4.3.5, we know that the boundary has length greater than  $r$ . Every face of a polycyclic realization of  $G$  yields a cycle of length  $r$  in  $G$ . Take a polycyclic realization  $P$  of  $G$  and consider the homomorphism  $\phi$  from  $P$  to  $\{r, q\}$ . Every cycle of length  $r$  in  $G$  determines, under the mapping  $\phi$ , a face  $F$  in  $\{r, q\}$ . Since any boundary has length greater than  $r$ , the face  $F$  corresponds to an interior face in  $P$ . Therefore, one has a one-to-one correspondence between interior faces of a polycyclic realization of  $G$  and cycles of length  $r$  in  $G$ . So, the graph  $G$  determines completely the polycyclic realization.  $\square$

Theorem 4.3.6 is an analog of Steinitz theorem for 3-connected planar graphs.

## 4.4 Angles and curvature

Recall that the regular tiling  $\{r, q\}$  lives on  $X = \mathbb{S}^2$ ,  $\mathbb{R}^2$ , or  $\mathbb{H}^2$  according to whether parameters  $(r, q)$  are elliptic, parabolic, or hyperbolic. The  $r$ -gons are regular in  $X$  and their curvature is  $2r\alpha(2, r, q)$ .

A set  $D$  in  $X$  is called *convex* if, for any two points  $x, y \in D$ , the geodesic joining  $x$  to  $y$  is contained in  $D$ . (Note that there are other definitions of convexity in hyperbolic space; see, for example, [GaSo01].) An  $(r, q)$ -polycycle is called *convex* if its image in

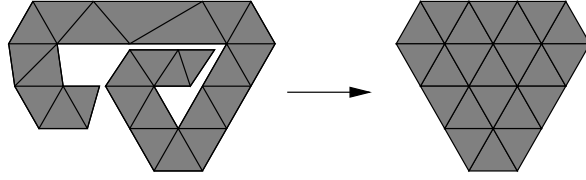


Figure 4.3: A convex non-proper  $(3, 6)$ -polycycle and its image in  $\{3, 6\}$

$\{r, q\}$  is convex. See on Figure 4.3 a convex  $(r, q)$ -polycycle, which is not proper. The only convex  $(r, 3)$ -polycycles are  $r$ -gon and  $\{r, 3\}$ . This is because, if a vertex  $v \in \{r, 3\}$  is contained in two  $r$ -gons  $F_1$  and  $F_2$ , then one can find two vertices  $v_1 \in F_1$  and  $v_2 \in F_2$  such that the geodesic between  $v_1$  and  $v_2$  pass by the third  $r$ -gon.

**Theorem 4.4.1** *Let  $P$  be an outerplanar  $(r, q)$ -polycycle. Then  $P$ , seen as a  $(r, 2q - 2)$ -polycycle, is convex and proper.*

**Proof.** Consider a face  $F$  in  $P$ . Starting with  $Dec(P)_0 = F$ , the finite  $(r, q)$ -polycycle  $Dec(P)_{n+1}$  is formed by  $Dec(P)_n$  and all faces of  $P$  sharing an edge with  $Dec(P)_n$ .  $Dec(P)_n$  and  $P$  are outerplanar  $(r, q)$ -polycycles; denote by  $\phi$  the cell-homomorphism of  $P$  into  $\{r, 2q - 2\}$ .

Every vertex of  $Dec(P)_n$  is contained into at most  $q - 1$   $r$ -gons; hence, the interior angle in the image  $\phi(Dec(P)_n)$  is at most  $\pi$ . This is a necessary and sufficient condition for the image  $\phi(Dec(P)_n)$  to be convex (see, for example, [GaSo01, Lemma 3.1]). Therefore, the image of the boundary of  $Dec(P)_n$  in  $\{r, 2q - 2\}$  is a not self-intersecting curve and  $Dec(P)_n$ , considered as a  $(r, 2q - 2)$ -polycycle, is proper.

If  $x$  and  $y$  are two points in  $\phi(P)$ , then there exists an integer  $n_0$  such that  $x, y \in \phi(Dec(P)_{n_0})$ . The geodesic  $d$  between  $x$  and  $y$  is included in  $\phi(Dec(P)_{n_0})$  and so, just as well in  $\phi(P)$ . If  $P$  is not proper, then there exist two distinct vertices  $v, v'$  (or edges, faces) of  $P$ , whose image in  $\{r, q\}$  coincide. There exists an integer  $n_0$  such that  $v, v' \in Dec(P)_{n_0}$ . But  $Dec(P)_{n_0}$  is proper; so, their images in  $\{r, q\}$  do not coincide.  $\square$

In the proof of above theorem, we need to use finite polycycles because infinite polycycles can have an infinity of boundaries.

**Theorem 4.4.2** *Let  $P$  be an outerplanar  $(3, q)$ -polycycle; then  $P$  is a proper  $(3, q + 2)$ -polycycle.*

**Proof.** By proof of Theorem 4.4.1, one can assume, without loss of generality, that  $P$  is finite. Denote by  $\phi$  the cell-homomorphism into  $\{3, q + 2\}$  and assume further that  $P$  is not a proper  $(3, q + 2)$ -polycycle. Then one can find two vertices  $v, v'$  on the boundary of  $P$  with  $\phi(v) = \phi(v')$  and the image of the boundary path  $\mathcal{P} = (v_0 = v, v_1, \dots, v_{p-1}, v_p = v')$  by  $\phi$  being not self-intersecting.  $\phi(\mathcal{P})$  defines a finite  $(3, q + 2)$ -polycycle, denoted by  $P'$ . Since  $P$  was originally a  $(3, q)$ -polycycle, the boundary vertices of  $P'$  are of degree at least 4, except, possibly, the vertex  $\phi(v) = \phi(v')$ . Denote by  $v_i$  the number of boundary vertices of  $P'$  of degree  $i$  different from  $\phi(v)$  and by  $v_{int}$  the number of interior vertices. Denote by  $p_3$  the number of 3-gons of  $P'$ .

The number  $e$  of edges satisfies to:

$$2e = 1 + \sum_{i=4}^{q+2} v_i + 3p_3 = (\deg \phi(v)) + \sum_{i=4}^{q+2} i v_i + (q+2)v_{int},$$

which implies  $3p_3 - (q+2)v_{int} = (\deg \phi(v)) - 1 + \sum_{i=4}^{q+2} (i-1)v_i$ . Then Euler formula  $v - e + f = 2$  with  $v = 1 + v_{int} + \sum_{i=1}^{q+2} v_i$  and  $f = 1 + p_3$  gives:

$$p_3 = qv_{int} + \sum_{i=4}^{q+2} \left(\frac{i}{2} - 1\right)v_i + \frac{\deg \phi(v)}{2}.$$

Eliminating  $p_3$ , one gets:

$$0 = (2q-2)v_{int} + \sum_{i=4}^{q+2} \left(\frac{i}{2} - 2\right)v_i + \frac{\deg \phi(v)}{2} + 1 > 1,$$

which is impossible.  $\square$

Remark, that already for  $p_3 = 7$ , there are outerplanar  $(3, 4)$ - and  $(3, 5)$ -polycycles which remain helices in  $\{3, 5\}$ ,  $\{3, 6\}$ , respectively. A *fan of  $(q-1)$   $r$ -gons* with  $q$ -valent common (boundary) vertex, is an example of outerplanar  $(r, q)$ -polycycle which is a proper non-convex  $(r, 2q-3)$ -polycycle.

We now consider another geometric viewpoint on  $(r, q)$ -polycycles. In the above consideration, the curvature was uniform and the triangles were viewed as embedded into a surface of constant curvature. Consider now the curvature to be constant, equal to zero, in the triangle itself and to be concentrated on the vertices, where  $r$ -gons meet.

The  $r$ -gons are now regular  $r$ -gons and the angle at its vertices is  $\frac{r-2}{r}\pi$ . Consider a point  $A$ , where  $q$   $r$ -gons meet. The curvature of  $A$  is the difference between  $2\pi$  and the sum of the angles of the  $r$ -gons, i.e.,  $2\pi - q\frac{r-2}{r}\pi$ . The total curvature of the  $(r, q)$ -polycycle is then:

$$v_{int}(2\pi - q\frac{r-2}{r}\pi) = v_{int}\frac{\pi}{r}(2(r+q) - rq).$$

It is different from the curvature defined above in this section, since boundary vertices contribute differently to it. If  $(r, q)$  is elliptic, parabolic, hyperbolic, then the curvature of interior vertices is positive, zero, negative, respectively.

We will use this curvature only for non-extensible polycycles in Section 8.2, and it will be only a counting, i.e., combinatorial, argument. However, the above curvature, concentrated on points, can be made geometric. This is the subject of Alexandrov theory (see, for example, [Ale50]).

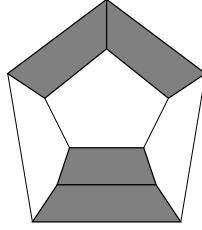
## 4.5 Polycycles on surfaces

We now present an extension of the notion of  $(r, q)$ -polycycle which concerns maps on surfaces. Given integers  $r, q \geq 3$ , an  $(r, q)$ -*gen-polycycle* is a 2-dimensional surface pasted together out of  $r$ -gons, so that the degree of interior vertices are equal to  $q$  and the degree of boundary vertices are within  $[2, q]$ .

A formal definition is the following: an  $(r, q)_{gen}$ -polycycle is a non-empty 2-connected map on surface  $S$  with faces partitioned in two non-empty sets  $F_1$  and  $F_2$ , so that it holds:

- (i) all elements of  $F_1$  (called *proper faces*) are combinatorial  $r$ -gons;
- (ii) all elements of  $F_2$  (called *holes*) are pair-wisely disjoint, i.e., have no common vertices;
- (iii) all vertices have degree within  $\{2, \dots, q\}$  and all *interior* (i.e., not on the boundary of a hole) vertices are  $q$ -valent.

Condition (ii) is here to forbid, for a vertex or an edge, to belong to more than one hole. This condition is not necessary for  $(r, q)$ -polycycle, since the simple connectedness and the 2-connectedness imply it. An example of a map, which does not satisfy it, is shown below:



An  $(r, q)_{gen}$ -polycycle, which is simply connected, is, in fact, an  $(r, q)$ -polycycle, i.e., it can be drawn on the plane and the holes became exterior in this drawing. Some  $(r, q)_{gen}$ -polycycle can be drawn on the plane, for example, half of those in Theorem 4.5.1. The theory of coverings, presented in Section 1.2, applies to this setting. The universal cover of an  $(r, q)_{gen}$ -polycycle is, by definition, simply connected and so, it is an  $(r, q)$ -polycycle.

**Theorem 4.5.1** *For  $r, q \leq 4$ , the list of  $(r, q)_{gen}$ -polycycles, which are not  $(r, q)$ -polycycles, consists of the following four infinite series:*

1.  *$Prism_m$ ,  $m \geq 2$  (on  $\mathbb{S}^2$ , with two  $m$ -gons seen as holes) and their non-orientable quotients, for  $m \geq 2$  even (on projective plane, with one hole),*
2.  *$APrism_m$ ,  $m \geq 2$  (on  $\mathbb{S}^2$ , with two  $m$ -gons seen as holes) and their non-orientable quotients, for  $m \geq 2$  odd (on projective plane, with one hole).*

**Proof.** The universal cover of such a polycycle is an  $(r, q)$ -polycycle with a non-trivial group of fixed-point-free automorphisms. The list of  $(r, q)$ -polycycles for  $r, q \leq 4$  is known (see Section 4.2). Inspection of this list gives only the infinite polycycles  $Prism_\infty = P_2 \times P_{\mathbb{Z}}$  and  $APrism_\infty = Tr_{\mathbb{Z}}$ . Their orientable quotients are: the infinite series of prisms  $Prism_m$  ( $m \geq 2$ ), the infinite series of antiprisms  $APrism_m$  ( $m \geq 2$ ) and the non-orientable quotients (with respect to central symmetry) of  $Prism_m$ , for  $m$  even, and of  $APrism_m$ , for  $m$  odd.  $\square$

The two dualities, inner and outer, extend to this setting. For example, one has equalities:

$$Inn^*(\text{snub } Prism_m) = APrism_m \quad \text{and} \quad Inn^*(\text{snub } APrism_m) = \text{snub } Prism_m.$$

In general, an  $(r, q)_{gen}$ -polycycle does not admit homomorphism to  $\{r, q\}$ , since  $(r, q)_{gen}$ -polycycles are not simply connected. But, sometimes, such homomorphism exists, see

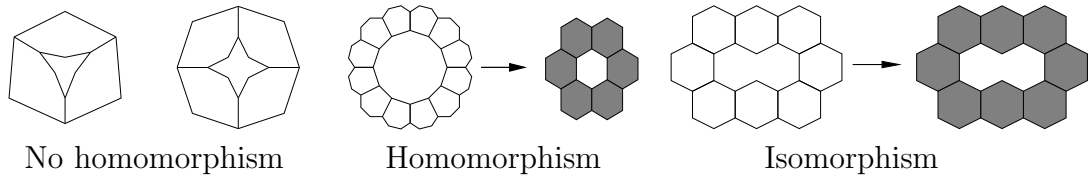


Figure 4.4: Some  $(6, 3)_{gen}$ -polycycles and their homomorphisms to  $\{6, 3\}$  when they exist

Figure 4.4. An  $(r, q)$ -map is a particular case of  $(r, q)_{gen}$ -polycycle, such that every vertex has degree  $q$ .

Finally, we mention two other relatives of finite  $(r, q)$ -polycycles. See [ArPe90] and references there (mainly authored by Perkel) for the study of *strict polygonal* graphs, i.e., graphs of girth  $r \geq 3$  and vertex-degree  $q$ , such that any path  $P_3$  (with two edges) belongs to a unique  $r$ -circuit of the graph. See [BrWi93, pages 546–547] for information on *equivelar* polyhedra, i.e., polyhedral embeddings with convex faces, of  $(r, q)$ -map into  $\mathbb{R}^3$ . So, in both these cases graphs are  $q$ -valent, have girth  $r$ , Euler-Poincaré characteristic  $v - e + f = \frac{v(6-r)}{2r}$  and coincide with Platonic polyhedra in the case of genus 0. Recall that, for an  $(r, q)$ -polycycle  $P$ , any non-boundary path  $P_3$  belongs to a unique  $r$ -circuit.



# Chapter 5

## Polycycles with given boundary

The  $(r, q)$ -*boundary sequence* of a finite  $(r, q)$ -polycycle  $P$  is the sequence  $b(P)$  of numbers enumerating, up to a cyclic shift or reversal, the consecutive degrees of vertices incident to the exterior face. For earlier applications of this (and other) codes, see [HeBr87, BCC92, HLZ96, DeGr99b, CaHa98, DFG01].

Given a  $(r, q)$ -boundary sequence  $b$ , a plane graph  $P$  is called a  $(r, q)$ -*filling* of  $b$  if  $P$  is a  $(r, q)$ -polycycle such that  $b = b(P)$ .

In this chapter we consider the unicity of those  $(r, q)$ -fillings and algorithms used for their computations.

### 5.1 The problem of uniqueness of $(r, q)$ -fillings

By inspecting the list of  $(r, q)$ -polycycles for  $(r, q) = (3, 3)$ ,  $(3, 4)$  or  $(4, 3)$  in Section 4.2 we find that the  $(r, q)$ -boundary sequence of an  $(r, q)$ -polycycle determines it uniquely. We expect that for any other pair  $(r, q)$  this is not so.

We show that the value  $r = 3, 4$  are the only ones, such that the  $(r, 3)$ -boundary sequence always define its  $(r, 3)$ -filling uniquely. Note that a  $(r, q)$ -polycycle which is not unique filling of its boundary is, necessarily, a helicene. Some examples of non-uniqueness of  $(r, 3)$ -filling are cases of boundaries  $b$ , admitting an  $(r, 3)$ -filling  $P$  with the symmetry group of  $b$  being larger than the symmetry group of  $P$ , implying the existence of several different  $(r, 3)$ -fillings. However, as the length of the boundary increase, the number of possibilities grows, see [DeSt06].

**Theorem 5.1.1** *For any  $r \geq 5$ , there is a  $(r, 3)$ -boundary sequence  $b$ , such that there exist  $(r, 3)$ -fillings  $P$  and  $P'$  with  $P \neq P'$  and  $b(P) = b(P') = b$ . For instance:*

(i) *If  $r = 5$ , then such example is given by  $b_5 = u3u3^4u3u3^4$  with  $u = 3232323$  of length 38 (see Figure 5.1).*

(ii) *If  $r \geq 6$ , then such example is given by*

$$b_r = u3^{r-1}u2^{r-6}u3^{r-1}u2^{r-6} \text{ with } u = (32^{r-4})^{r-1}3$$

*of length  $4r^2 - 12r + 2$ . Amongst vertices of this boundary,  $6r - 2$  vertices are of degree 3 and the remaining ones are of degree 2 (see Figure 5.2).*

*The  $(r, 3)$ -boundary sequence  $b_r$  can be filled by  $4r$   $r$ -gons in two ways, which are obtained one from the other by mirror.*

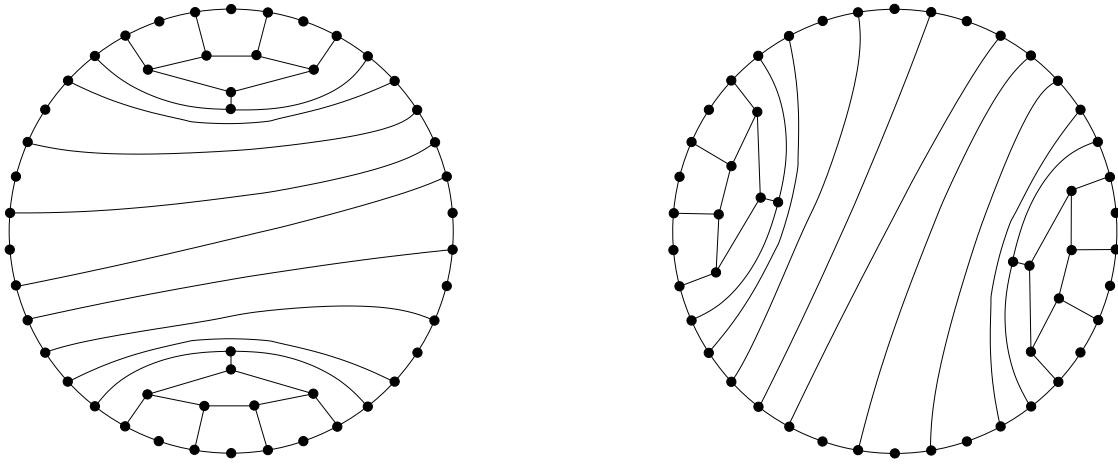


Figure 5.1: Two different (but isomorphic as maps)  $(5,3)$ -fillings of the same  $(5,3)$ -boundary

**Proof.** For any of the boundary sequences indicated in the theorem, the symmetry group is  $C_{2\nu}$  of size 4. Furthermore, the fillings on Figures 5.1 and 5.2, for  $p = 5, 6, 7$ , have symmetry  $C_2$ , which is a group of order 2. This is, in fact, true for any  $b_r$  with  $r \geq 5$ . So, the  $(r, 3)$ -boundary  $b_r$  has at least two fillings, which are isomorphic as maps but different. It proves that the  $(r, 3)$ -boundary sequence  $b_r$  does not define uniquely its  $(r, 3)$ -filling.  $\square$

The main difficulty of above theorem consists in finding the  $(r, 3)$ -boundary sequence  $b_r$ . It seems likely that our examples are minimal with respect to the number of  $r$ -gons of their corresponding fillings.

**Remark 5.1.2** The  $(3, 5)$ -boundary sequence  $(43445544345)^2$  admits two different  $(3, 5)$ -fillings (by 36 3-gons and 30 vertices) shown on Figure 5.3. Those fillings are isomorphic and have only symmetry  $C_2$  while the boundary has symmetry  $C_{2\nu}$ , like in Theorem 5.1.1.

The  $(3, 5)$ -boundary sequence  $(34345)^2 5^2 (34345)^2 5^2$  admits two different  $(3, 5)$ -fillings (by 34 3-gons and 30 vertices) shown on Figure 5.4. Those fillings are non-isomorphic and have the same symmetry as the boundary, i.e.,  $C_2$ . This  $(3, 5)$ -boundary sequence might be minimal for the number of 3-gons.

In the case of  $(5, 3)$ -polycycles, for every given number we have an example of a  $(5, 3)$ -boundary sequence, which admits exactly that number of fillings. The statement and the proof of this theorem uses elementary polycycles, presented in Chapter 7 (especially,  $E_1$ ,  $C_1$  and  $C_3$  from Figure 7.2).

**Theorem 5.1.3** The  $(5, 3)$ -boundary  $b(n) = 223^{5n+1} 223^{5n+3} 223^{5n+1} 223^{5n+3}$  admits exactly  $n+1$  different  $(5, 3)$ -fillings. Each such filling corresponds to a number  $k$ ,  $0 \leq k \leq n$ , where the  $k$ -th filling is obtained by taking two elementary  $(5, 3)$ -polycycles  $E_1$ , gluing them and adding to four open edges of  $E_1 + E_1$ , respectively, chains of  $k$ ,  $n - k$ ,  $k$  and  $n - k$  elementary polycycles  $C_1$ .

**Proof.** One needs to prove only that there is no more than those  $n + 1$  fillings. First, since all runs of two are 22, the only possible elementary  $(5, 3)$ -polycycles are  $E_1$ ,  $C_1$

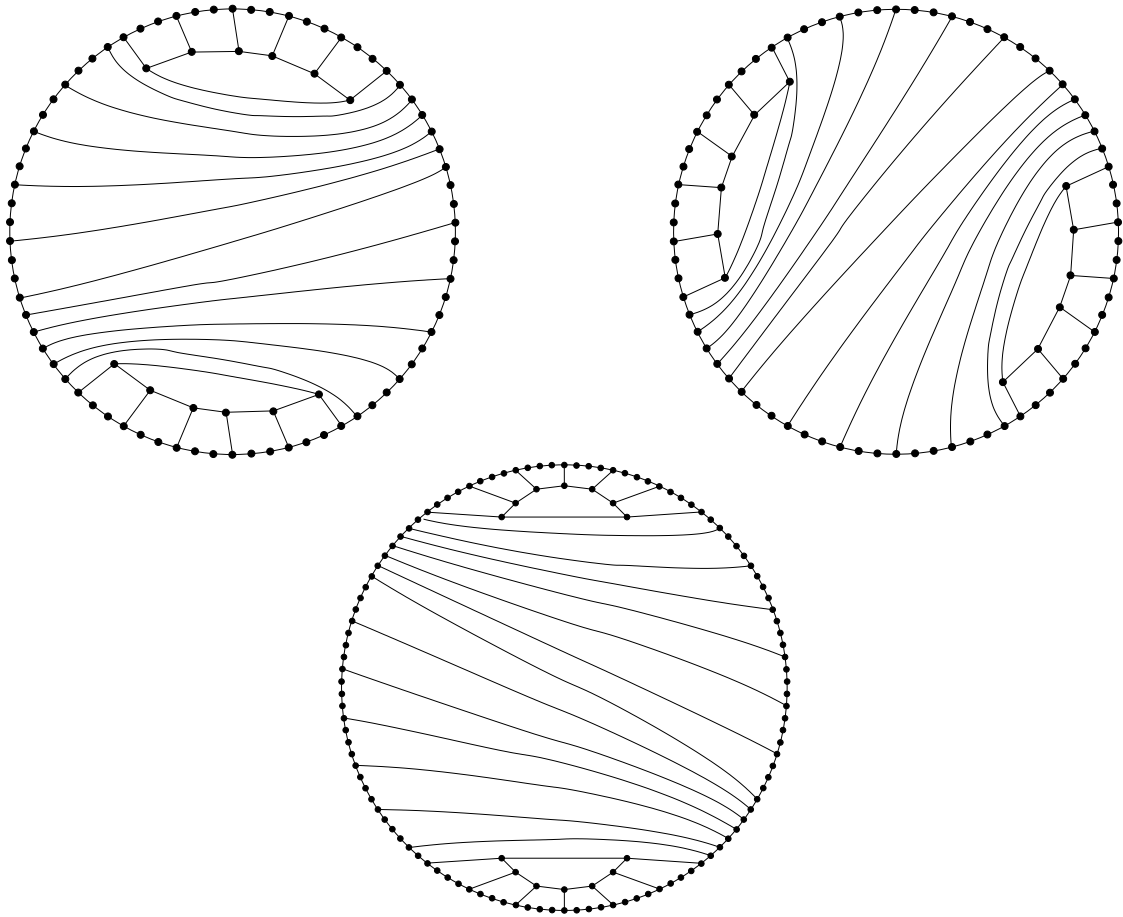


Figure 5.2: Two different (but isomorphic as maps)  $(6,3)$ -fillings of the same  $(6,3)$ -boundary; the left one and the lower one are the first cases  $r = 6, 7$  of a series of  $(r,3)$ -fillings, which are not defined by their boundaries

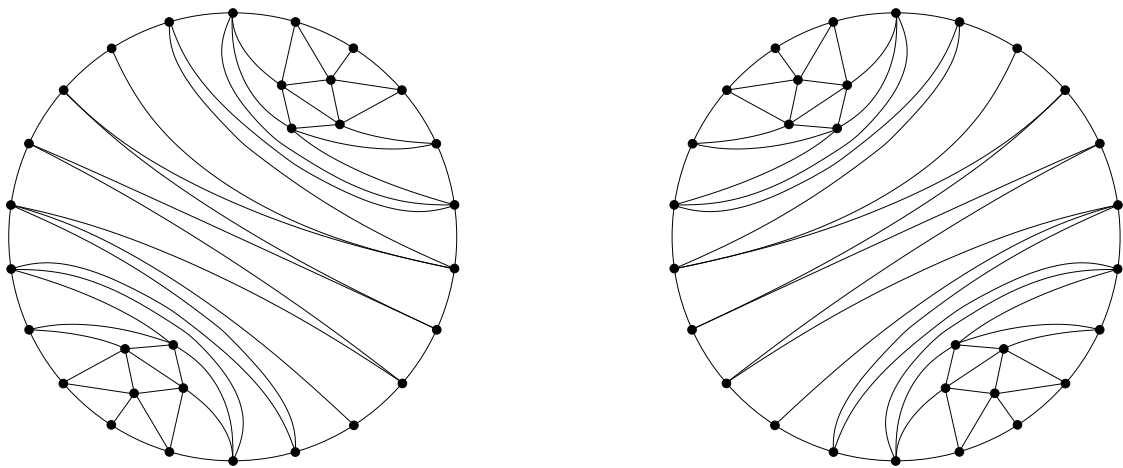


Figure 5.3: Two different (but isomorphic as maps)  $(3,5)$ -fillings of the same boundary

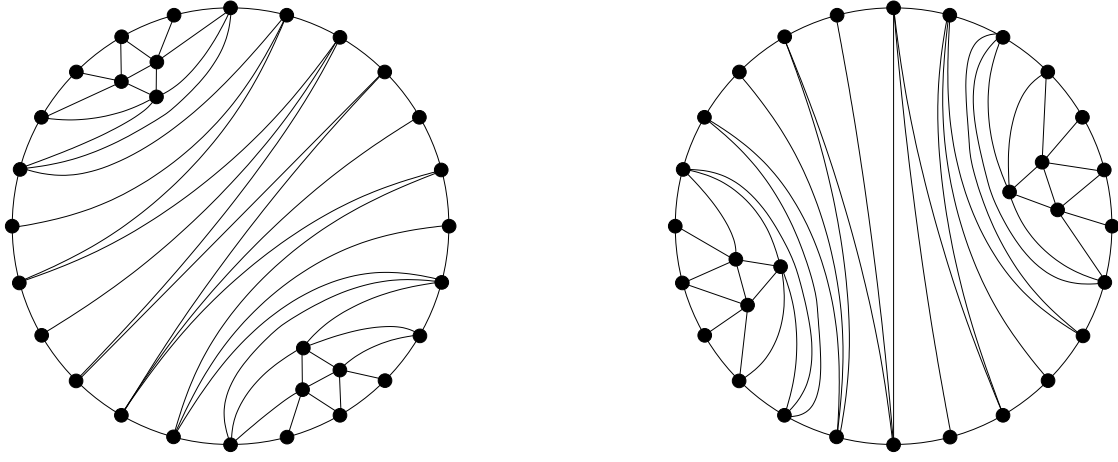


Figure 5.4: Two different non-isomorphic  $(3, 5)$ -fillings (with symmetry  $C_2$ ) of the same boundary with symmetry  $C_2$

or  $C_3$ . Secondly, since the  $(5, 3)$ -boundary has exactly 4 runs of 2, the total number of  $(5, 3)$ -polycycles  $E_1$  and  $C_3$  is 2.

The addition of the  $(5, 3)$ -polycycle  $C_1$  to an existing  $(5, 3)$ -polycycle, adds the symbol  $3^5$  at two emplacement of the  $(5, 3)$ -boundary sequence. The three possible cases  $E_1 + E_1$ ,  $E_1 + C_3$  and  $C_3 + C_3$  correspond, respectively, to  $(5, 3)$ -boundary sequences  $223^1 223^3 223^1 223^3$ ,  $223^2 223^4 223^1 223^4$  and  $223^2 223^5 223^2 223^5$ . So, the only possibility, that agrees modulo 5, is  $E_1 + E_1$ . It is easy to see that there is no polycycle  $C_1$  between two polycycles  $E_1$  and that the number of polycycles  $C_1$ , inserted on every part of the four open edges (i.e., with 2-valent end vertices), is  $k$ ,  $n - k$ ,  $k$  and  $n - k$ .  $\square$

**Conjecture 5.1.4** (i) If the number of  $r$ -gons of  $(r, 3)$ -polycycle is strictly less than  $4r$ , then the  $(r, 3)$ -boundary sequence defines it uniquely. It holds for  $r = 6$  ([GHZ02]) and for  $r = 5$  ([DeSt06]).

(ii) Let  $b_r$  be the boundary for the example defined in Theorem 5.1.1; we expect that it does not admit neither  $(r', 3)$ -filling with  $r' > r$ , nor  $(r, q)$ -filling with  $q > 3$ .

Call a  $(r, q)$ -boundary sequence *ambiguous* if it admit at least two different  $(r, q)$ -fillings. Call it *irreducible*, if its  $(r, q)$ -filling does not contain, as induced polycycle, the  $(r, q)$ -fillings of another ambiguous  $(r, q)$ -boundary sequences.

The number of irreducible ambiguous  $(5, 3)$ -boundary sequences is 0, 1, 3, 17, for  $p_5 < 20, 20, 21, 22$ , respectively (see [DeSt06], where such  $(5, 3)$ -polycycles are called *equi-boundary polypentagons*).

The ambiguous  $(5, 3)$ -boundary sequence for  $p_5 = 20$ , is  $(2323233^5 2323233^2)^2$ . The irreducible ambiguous  $(5, 3)$ -boundary sequences with  $p_5 = 21$  are:

| $b$                                         | $ b $ | $Aut(b)$ | Nr. of fillings | Isomorphic fillings |
|---------------------------------------------|-------|----------|-----------------|---------------------|
| $3^2 232323^6 2323^4 2323^6 232323$         | 35    | $C_s$    | 2               | yes                 |
| $3^2 232323^6 23^2 2^3 4 232323^6 232323$   | 39    | $C_1$    | 2               | no                  |
| $3^2 232323^7 2^3 2^3 23^3 232323^6 232323$ | 39    | $C_1$    | 2               | no                  |

Here  $|b|$  is the length of the sequence,  $Aut(b)$  is its automorphism group and we indicate if the obtained fillings are isomorphic. On Figure 5.5, a  $(6, 3)$ -polycycle is presented,

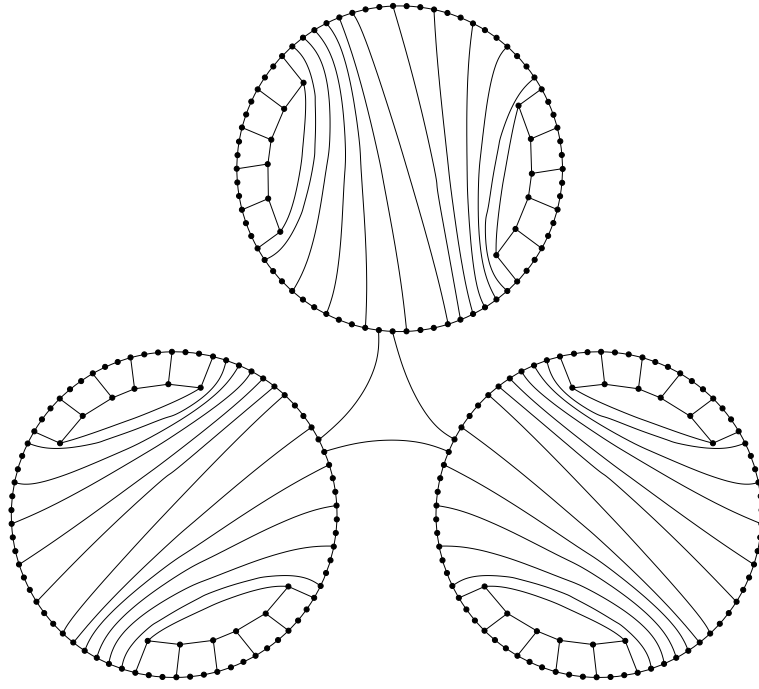


Figure 5.5: Several non-isomorphic  $(6, 3)$ -fillings of the same  $(6, 3)$ -boundary are obtained by different  $(6, 3)$ -fillings of above 3 components

whose  $(6, 3)$ -boundary sequence admits eight different  $(6, 3)$ -fillings. More generally, by aggregating the examples, found in Theorem 5.1.1, one can obtain an  $(r, 3)$ -boundary, admitting an arbitrary large number of fillings. Furthermore, by adding one  $r$ -gon to an example, found in Theorem 5.1.1, one can obtain  $(r, 3)$ -boundaries, admitting two non-isomorphic  $(r, 3)$ -fillings.

Note that if two  $(r, q)$ -polycycles have the same  $(r, q)$ -boundary, then their image under the cell-homomorphism in  $\{r, q\}$  is the same. Moreover, in [Gra03] it is proved that if the image of a  $(6, 3)$ -polycycle does not triply cover some point, then the  $(6, 3)$ -boundary sequence determine this  $(6, 3)$ -polycycle uniquely.

## 5.2 $(r, 3)$ -filling algorithms

The algorithmic problem treated here is: given a  $(r, 3)$ -boundary, find all possible  $(r, 3)$ -fillings of it.

**Theorem 5.2.1** *Let  $P$  be a  $(r, 3)$ -polycycle. Denote by  $x$  the number of interior vertices of  $P$  and by  $p_r$  the number of  $r$ -gonal faces in  $P$ . Denote by  $v_2, v_3$  the number of vertices of degree 2, 3, respectively, on the  $(r, 3)$ -boundary; then it holds:*

$$\begin{cases} p_r - \frac{x}{2} &= 1 + \frac{v_3}{2} \\ rp_r - 3x &= v_2 + 2v_3 \end{cases} \quad (5.1)$$

Moreover, it holds:

- (i) if  $r \neq 6$ , then  $x = \frac{2(v_2 - r) - (r - 4)v_3}{r - 6}$  and  $p_r = \frac{v_2 - v_3 + 5}{r - 6}$ .
- (ii) if  $r = 6$ , then  $v_2 = v_3 + 6$ .

**Proof.** The number of edges  $e$  satisfies to  $2e = v_2 + v_3 + rp_r = 2v_2 + 3v_3 + 3x$ , which implies  $rp_r - 3x = v_2 + 2v_3$ . Then Euler formula  $v - e + f = 2$  with  $v = v_2 + v_3 + x$  and  $f = 1 + p_r$  implies  $p_r - \frac{x}{2} = 1 + \frac{v_3}{2}$ .

The linear system (5.1) has a unique solution if and only if  $r \neq 6$ , thereby proving (i). (ii) is obvious.  $\square$

Actually, for  $r = 6$  also the  $(r, 3)$ -boundary determines the number of  $r$ -gons (see [GHZ02, BDvN06]).

The basic idea of the  $(r, 3)$ -filling algorithm is the following. Given a  $(r, 3)$ -boundary  $b$  and two consecutive vertices  $x$  and  $y$  of degree 3 on it, consider all possible ways to add an  $r$ -gonal face to this pair of vertices. When adding an  $r$ -gonal face, there are several possibilities (illustrated on Figure 5.6):

- either the new  $r$ -gon does not split the  $(r, 3)$ -boundary into different components,
- or it splits the  $(r, 3)$ -boundary into two, or more, components.

Given one pair of vertices  $x$  and  $y$ , all cases should be considered. Then, the algorithm should be reapplied to the remaining boundaries, until one obtains a  $(r, 3)$ -polycycle.

The order, in which cases are considered, affects the speed of computation. We choose the pair  $x, y$  with the smallest number of possibilities of extension.

In particular, if the  $(r, 3)$ -boundary sequence contains the pattern  $2^{r-1}$  or  $2^{r-2}$ , then there is a unique way of adding an edge; so, one obtains a unique smaller problem (see Figure 5.7).

Another speedup consists in showing that a  $(r, 3)$ -boundary  $b$  does not admit any  $(r, 3)$ -fillings. Two criteria are possible:

- Use Theorem 5.2.1 to compute the number of interior vertices and faces. If they are negative or non-integer, then the  $(r, 3)$ -boundary is non-extensible. This is a global criterion.
- If a pair of consecutive vertices of valency 3 on the  $(r, 3)$ -boundary does not admit any extension by an  $r$ -gon, i.e., its distance is lower than  $r - 1$ , then the  $(r, 3)$ -boundary is non-extensible. This is a local criterion.

By using those methods, one can find all  $(r, 3)$ -fillings of a given  $(r, 3)$ -boundary. The running time is, most likely, non-polynomial; if the length of the  $(r, 3)$ -boundary increase, the number of cases to consider become very large and the efficiency of the above criteria is limited. Nevertheless, if  $r \neq 6$ , the algorithm is guaranteed to terminate, since then one knows how many  $r$ -gons will occur. If one wants to check, whether a  $(r, q)$ -boundary corresponds to a proper  $(r, q)$ -polycycle, then this is easier. The  $(r, q)$ -boundary sequence specify a path in  $\{r, q\}$ , this path has to be closed and this is an easily checked condition. The second and sufficient condition is that the path has to be non self-intersecting. Both conditions can be checked in polynomial time.

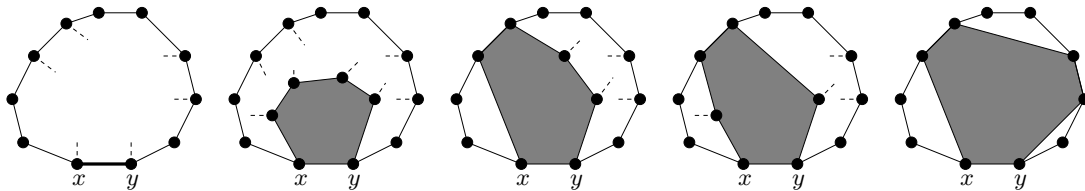


Figure 5.6: Some examples of possible ways to add a 6-gon between two vertices  $x$  and  $y$  of valency 3 on the  $(6, 3)$ -boundary

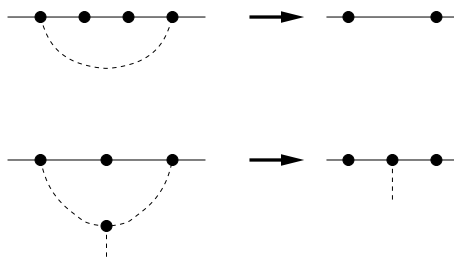


Figure 5.7: The unique completion cases for  $r = 4$



# Chapter 6

## Symmetries of polycycles

Remind that the *automorphism group*  $Aut(P)$  of an  $(r, q)$ -polycycle  $P$  is the group of automorphisms of the plane graph preserving the set of interior faces (see Section 4.1). Call a polycycle  $P$  *isotoxal*, *isogonal*, or *isohedral* if  $Aut(P)$  is transitive on edges, vertices, or interior faces, respectively. In this chapter we first consider the possible automorphism groups of an  $(r, q)$ -polycycle, then we list all isogonal or isohedral polycycles for elliptic  $(r, q)$  and present a general algorithm for their enumeration. We also present the problem of determining all isogonal and isohedral  $(r, q)_{gen}$ -polycycles.

### 6.1 Automorphism group of $(r, q)$ -polycycles

If an  $(r, q)$ -polycycle  $P$  is finite, then it has a single boundary and  $Aut(P)$  consists only of rotations and mirrors around this boundary. So, its order divides  $2r$ ,  $4$  or  $2q$ , depending on what  $Aut(P)$  fixes: the center of an  $r$ -gon, the center of an edge or a vertex.

None of  $(3, 3)$ -,  $(3, 4)$ -,  $(4, 3)$ -polycycles, but almost all  $(r, q)$ -polycycles for any other  $(r, q)$ , have trivial  $Aut(P)$ .

The number of *chiral* (i.e., with  $Aut(P)$  containing only rotations and translations) proper  $(5, 3)$ -,  $(3, 5)$ -polycycles is 12, 208 (amongst, respectively, all 39, 263.)

Given an  $(r, q)$ -polycycle  $P$ , consider the cell-homomorphism  $\phi$ , presented in Section 4.3, from  $P$  to  $\{r, q\}$ . It maps the group  $Aut(P)$  into  $Aut(\{r, q\}) = T^*(l, m, n)$ . The image  $\phi(Aut(P))$  consists of automorphisms of  $\phi(P)$ . If  $P$  is a proper polycycle, then  $Aut(P)$  coincides with  $Aut(\phi(P))$ . Otherwise,  $Aut(P)$  is an extension of  $Aut(\phi(P))$  by the kernel of this homomorphism.

Only  $r$ -gons and non-Platonic plane tilings  $\{r, q\}$  are isotoxal; their respective automorphism groups are  $C_{r\nu}$  and  $T^*(2, r, q)$ . The group  $Aut(\{r, q\} - f)$  is  $C_{r\nu}$  in five Platonic cases; none is isotoxal, isogonal or isohedral polycycle, except of isohedral  $\{3, 3\} - f = (3, 3)$ -star.

We call the set of  $q$   $r$ -gons with a common vertex, the  $(r, q)$ -*star* of  $q$ -gons.

### 6.2 Isohedral and isogonal $(r, q)$ -polycycles

**Theorem 6.2.1** *Let  $P$  be an isohedral  $(r, q)$ -polycycle; then it holds:*

- (i)  *$P$  has the same number  $t$  of non-boundary edges for each its  $r$ -gon.*

- (ii) For  $t = 0, r$  or  $1$ , the polycycle  $P$  is, respectively,  $r$ -gon, non-elliptic  $\{r, q\}$ , or a pair of adjacent  $r$ -gons (with  $\text{Aut}(P) = C_{2\nu}$ ).
- (iii) If  $t = 2$ , then  $P$  is either a  $(r, q)$ -star, or an infinite outerplanar polycycle.
- (iv) If  $t \geq 3$ , then  $P$  is infinite.

**Theorem 6.2.2** (i) For a given pair  $(r, q)$ , the number of isohedral  $(r, q)$ -polycycles is finite. Moreover, it is bounded by a function depending only on  $r$ .

(ii) If  $P$  is an isogonal  $(r, q)$ -polycycle, then either it is  $r$ -gon, or non-elliptic  $\{r, q\}$ , or an infinite outerplanar polycycle and its outer dual  $\text{Out}^*(P)$  (considering  $P$  as an  $(r, q + 1)$ -polycycle) is an isohedral infinite  $(q + 1, r)$ -polycycle.

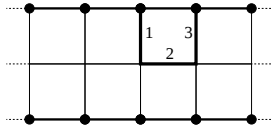
**Proof.** Consider an isohedral  $(r, q)$ -polycycle  $P$  and fix a face  $F$  in it. The automorphism group of an  $r$ -gon is the dihedral group  $C_{r\nu}$ ; the stabilizer  $\text{Stab}(F)$  of  $F$  in  $P$  is a subgroup of  $C_{r\nu}$ . Since  $C_{r\nu}$  is finite, one has a finite number of possibilities for  $\text{Stab}(F)$ . The face  $F$  is adjacent in  $P$  to  $t$   $r$ -gonal faces  $F_1, \dots, F_t$ . By isohedrality, one has, for every  $i$ , a transformation  $\phi_i$  of  $P$  that maps  $F$  to  $F_i$ . This transformation is defined up to an element of  $\text{Stab}(F)$ . Clearly, there are at most  $2r$  possible transformations  $\phi_i$ . One way to see it is that  $\phi_i$  is defined by the image of a flag  $(v, e, F)$  into a flag  $(v', e', F_i)$  and that there are  $2r$  such flags. So, the finiteness is established. Moreover, the number of choices for  $\text{Stab}(F)$  depends only on  $r$ ; so, the total number of choices is bounded by a function depending only on  $r$ .

If  $P$  is an isogonal  $(r, q)$ -polycycle, then either no vertex belongs to the boundary and we have no boundary, or every vertex belongs to the boundary and  $P$  is outerplanar. If  $P$  is outerplanar, then one can consider it as an  $(r, q + 1)$ -polycycle and so, the outer dual is well defined and isohedral.  $\square$

Given a pair  $(r, q)$ , above theorem gives that the set of isohedral  $(r, q)$ -polycycles is finite but it does not precise how we can enumerate them. Given an  $r$ -gon  $F$  of  $P$ , we specify transformation which maps  $F$  to adjacent  $r$ -gons to  $F$ . After those transformation are prescribed one checks if the coherency is satisfied of  $F$ . Simple connectedness assures us that those local conditions are actually global (see [Dre87], for the proofs). The actual enumeration is then done by computer using exhaustive enumeration schemes (see [Du07]).

**Theorem 6.2.3** For any  $r$ , there exists isohedral  $(r, 4)$ -polycycle with exactly one boundary edge on each  $r$ -gon.

**Proof.** Take an  $r$ -gon  $F$  and select  $r - 1$  edges. On every one of those edges define the line symmetry that maps the  $r$ -gon to its mirror along the edge; see below, for  $r = 4$ , the line symmetries along edges 1, 2 and 3:



The  $r$ -gon has  $r - 2$  interior vertices. All those transformations fit together around those vertices. So, they yield an isohedral  $(r, 4)$ -polycycle.  $\square$

For non-elliptic  $(r, q)$ , the practical representation of an isohedral  $(r, q)$ -polycycle is difficult, since the number of vertices at distance  $r$  from a given vertex grows very fast

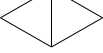
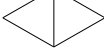
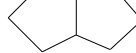
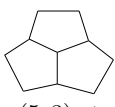
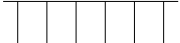
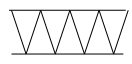
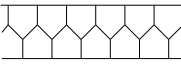
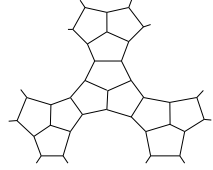
| $Aut(P) \backslash (r, q)$                        | (3, 3)                                                                                           | (3, 4)                                                                                                 | (4, 3)                                                                                              | (3, 5)                                                                                                                                                                                                             | (5, 3)                                                                                                                                                                                                                                                                 |
|---------------------------------------------------|--------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| $C_{r\nu}$<br>$\simeq T(2, 2, r)$                 | <br>3-gon       | <br>3-gon             | <br>4-gon          | <br>3-gon                                                                                                                        | <br>5-gon                                                                                                                                                                           |
| $C_{2\nu}$<br>$\simeq T(2, 2, 2)$                 |                 |                       |                    |                                                                                                                                  |                                                                                                                                                                                     |
| $C_{q\nu}$<br>$\simeq T(2, 2, q)$                 | <br>(3, 3)-star | <br>(3, 4)-star       | <br>(4, 3)-star    | <br>(3, 5)-star                                                                                                                  | <br>(5, 3)-star                                                                                                                                                                     |
| $pm11$<br>$\simeq T(2, 2, \infty)$                |                                                                                                  |                                                                                                        |                                                                                                     |                                                                                                                                                                                                                    |                                                                                                                                                                                     |
| $pmm2$<br>$= T^*(2, 2, \infty)$                   |                                                                                                  |                                                                                                        | <br>$Prism_\infty$ |                                                                                                                                                                                                                    |                                                                                                                                                                                                                                                                        |
| $pma2$<br>$= T(2, 2, \infty)$                     |                                                                                                  | <br>$APrism_\infty$ |                                                                                                     | <br>$APrism_\infty$<br><br>$APrism_\infty$ | <br><br> |
| $T^*(2, 3, \infty)$<br>$\simeq SL(2, \mathbb{Z})$ |                                                                                                  |                                                                                                        |                                                                                                     |                                                                                                                                                                                                                    |                                                                                                                                                                                   |

Figure 6.1: All 19 isohedral elliptic  $(r, q)$ -polycycles; only  $r$ -gons and  $Prism_\infty$ ,  $APrism_\infty$  are isogonal (the remaining  $9^{th}$  elliptic isogonal polycycle is given on the right-hand side of Figure 6.3)

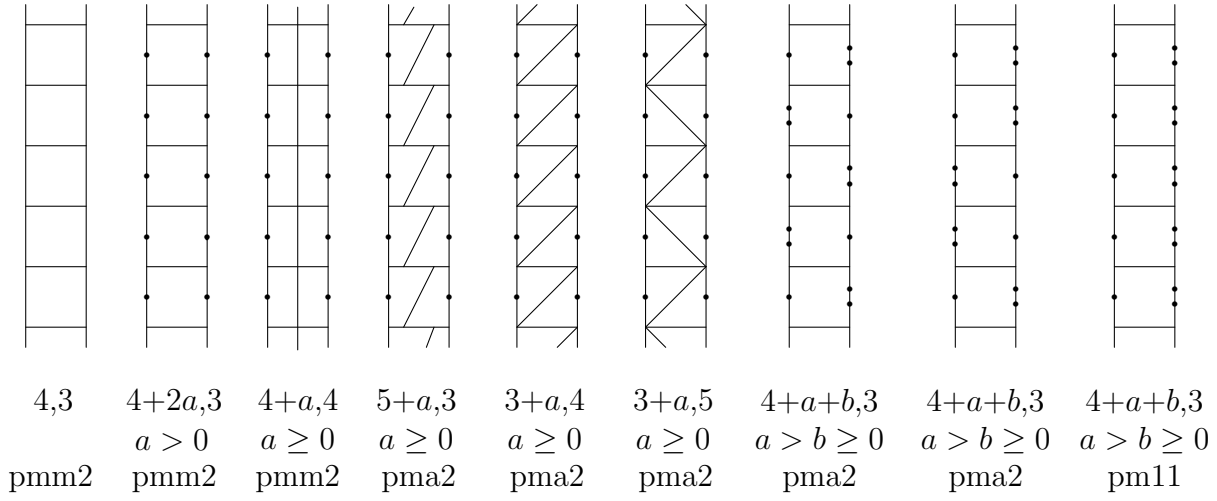
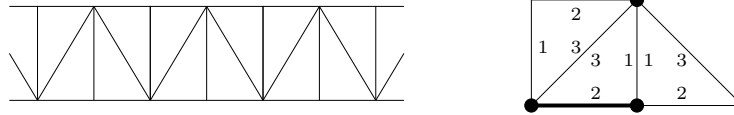


Figure 6.2: Conjecturally complete list of eight families of isohedral  $(r, q)$ -polycycles with a strip group of symmetry presented as decorated  $Prism_\infty$  (only 1st and 5th, for  $a = 0$ , are isogonal)

and we are led to draw smaller and smaller faces. The compressed presentation (see Theorems 6.2.5 and 6.2.6 below) will mimic the computer presentation of such polycycles: it presents one  $r$ -gon  $F$  and its adjacent  $r$ -gons  $F_i$ . Boundary edges and boundary vertices are boldfaced. The edges of  $F$  are marked by a number and the edges of the adjacent  $r$ -gons  $F_i$  have those numbers under a symmetry transformation (generally, non-unique) mapping  $F$  to  $F_i$ . The stabilizer  $Stab(F)$  of  $F$  is a point group, whose type is indicated under picture. See below a representation of an infinite  $(3, 5)$ -polycycle and its corresponding code:



A similar representation can be done for isogonal  $(r, q)$ -polycycles.

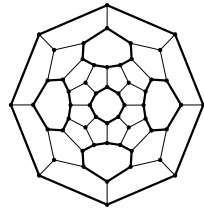
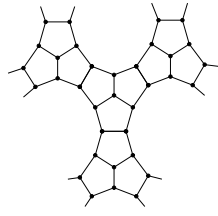
Another way to get a representation, is to take a quotient  $\tilde{P}$  of a  $(r, q)$ -polycycle  $P$  by a subgroup of  $Aut(P)$ .  $\tilde{P}$  might be easier to represent and  $P$  is then obtained by taking the universal cover of the  $(r, q)_{gen}$ -polycycle  $\tilde{P}$ . See on Figure 6.3 two examples of such description.

Using the algorithm of Theorem 6.2.2, in [DeSt00b], all elliptic isohedral polycycles were found (see Figure 6.1): 11 finite ones, 7 infinite ones with strip groups and a  $(5, 3)$ -polycycle with  $Aut(P) = T^*(2, 3, \infty)$ .

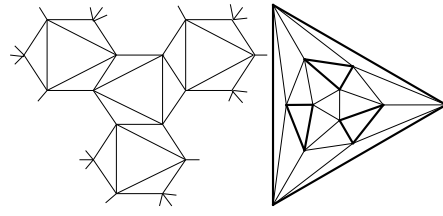
The enumeration of elliptic isogonal  $(r, q)$ -polycycles yields 9 polycycles: all three  $r$ -gons (as five polycycles),  $Prism_\infty$ ,  $APrism_\infty$  (as two polycycles) and the isogonal  $(3, 5)$ -polycycle represented on Figure 6.3.

We now list some existence and classification results for isohedral  $(r, q)$ -polycycles obtained by using the previous formalism.

**Remark 6.2.4** *If a  $(r, q)$ -polycycle is proper, then one can realize its group of combinatorial transformations as a group of isometries of its image in  $\{r, q\}$ . If the  $(r, q)$ -polycycle*



An isohedral  $(5,3)$ -polycycle of symmetry  $T^*(2,3,\infty)$



An isogonal  $(3,5)$ -polycycle of symmetry  $T(2,3,\infty)$

Figure 6.3: Two examples of infinite  $(r,q)$ -polycycles with, for each of them, a quotient  $(r,q)_{gen}$ -polycycle (strictly face-regular Nr. 58 and Icosahedron with boldfaced six, respectively, four holes)

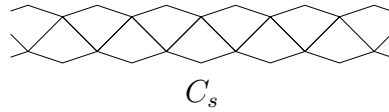
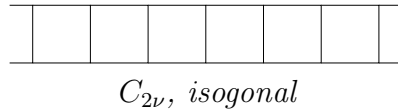
is a helicene, then this is not possible; see, for example, the infinite elliptic isohedral  $(r,q)$ -polycycles on Figure 6.1. Unfortunately, we do not know any method for checking if a given  $(r,q)$ -polycycle is proper or not.

**Theorem 6.2.5** All isohedral  $(3,q)$ -polycycles with  $q \geq 3$  are:

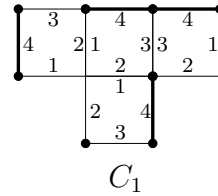
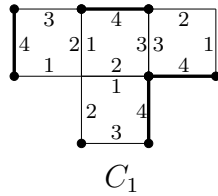
- (i) 3-gon (isogonal),  $\{3,q\}$  (isogonal), pair of adjacent 3-gons,  $(3,q)$ -star.
- (ii) For  $q \geq 4$ ,  $A\text{Prism}_\infty$  (isogonal) and, for  $q \geq 5$ , the infinite not isogonal  $(3,5)$ -polycycle from Figure 6.1.

**Theorem 6.2.6** All isohedral  $(4,q)$ -polycycles with  $q \geq 3$  are:

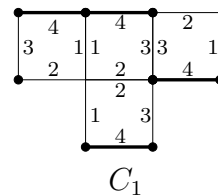
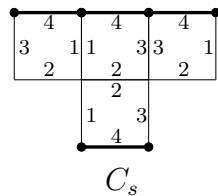
- (i) 4-gon (isogonal),  $\{4,q\}$  (isogonal), pair of adjacent 4-gons,  $(4,q)$ -star.
- (ii) For  $q \geq 3$ , respectively,  $q \geq 4$ , the following outerplanar  $(4,3)$ -polycycle, respectively,  $(4,4)$ -polycycle:



- (iii) For  $q \geq 4$ , respectively,  $q \geq 5$ , the following  $(4,q)$ -polycycles:



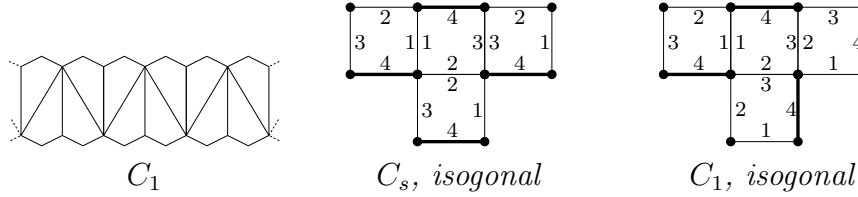
- (iv) If  $q \geq 4$  even, respectively,  $q \geq 6$  even, the following  $(4,q)$ -polycycles:



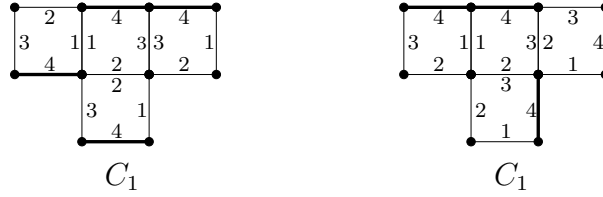
| $r \downarrow q \rightarrow$ | 3        | 4         | 5          | 6           | 7            | 8            |
|------------------------------|----------|-----------|------------|-------------|--------------|--------------|
| 3                            | 2, 0, 0  | 3, 1, 1   | 4, 2, 1    | 4, 3, 1     | 4, 6, 1      | 4, 11, 1     |
| 4                            | 3, 1, 1  | 6, 3, 1   | 9, 8, 3    | 11, 21, 3   | 11, 53, 3    | 13, 137, 3   |
| 5                            | 7, 0, 0  | 17, 0, 0  | 24, 0, 0   | 38, 5, 5    | 37, 13, 5    | 51, 19, 5    |
| 6                            | 12, 1, 1 | 45, 4, 3  | 67, 11, 3  | 130, 24, 3  | 123, 87, 20  | 196, 234, 20 |
| 7                            | 28, 0, 0 | 157, 0, 0 | 257, 0, 0  | 518, 0, 0   | 452, 0, 0    | 896, 60, 60  |
| 8                            | 58, 1, 1 | 486, 3, 1 | 894, 11, 6 | 2095, 35, 6 | 1781, 119, 6 | 3823, 367, 6 |

Table 6.1: Triples  $(x, y, z)$  of numbers  $x$  of isohedral,  $y$  of isogonal,  $z$  of isohedral and isogonal  $(r, q)$ -polycycles, different from  $r$ -gon and  $\{r, q\}$ , for  $r, q \leq 8$

(v) For  $q \geq 5$ , the following three outerplanar  $(4, 5)$ -polycycles:



(vi) For  $q \geq 7$ , the following two outerplanar  $(4, 7)$ -polycycles:



**Proof.** The proof is a case by case analysis. It is exactly the same as running the program; so, we refer to the program itself.  $\square$

Clearly,  $y$  and  $z$ , introduced in Table 6.1, are non-decreasing functions of  $q$  and  $z \leq \min(x, y)$ . From Theorem 6.2.5, it follows that if  $r = 3$  and  $q \geq 4$ , then  $z = 1$  and it is realized by  $A\text{Prism}_\infty$ , seen as a  $(3, q)$ -polycycle.

**Conjecture 6.2.7** (i) If  $r$  is odd, then  $y = z = 0$  for  $3 \leq q \leq r$ ,  $y = z > 0$  for  $q = r + 1$  and  $y > z > 0$ , otherwise.

(ii) If  $r$  is even, then  $y > z > 0$  for  $q \geq 4$  and  $y = z = 1$ , for  $q = 3$ ; it is realized by  $(r, 3)$ -cactus (infinite  $(r, 3)$ -polycycle obtained by growing from an  $r$ -gon, i.e., adding  $r$ -gon on  $\frac{r}{2}$  disjoint edges, see two decoration of the  $(6, 3)$ -cactus on Figure 6.3).

The computation of isohedral  $(r, q)$ -polycycles, presented in Table 6.1, shows that a full classification of them is hopeless. Note that the algorithm gives the list of isohedral  $(r, q)$ -polycycles but not their groups. It is possible to generate by computer a presentation of the group by generators and relations. But the groups, defined by generators and relations, are notorious in Group Theory (for even the simplest questions) to be *undecidable* (that is no algorithm can answer those questions in full generality). It makes the identification with known groups somewhat of an art. See below an isohedral  $(6, 3)$ -polycycle (obtained in [DeSt01] with many other examples), whose automorphism group  $\mathbb{Z}_3 \times T^*(\infty, \infty, \infty)$  is not a Coxeter group:

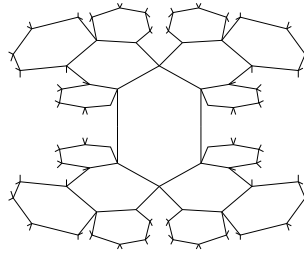
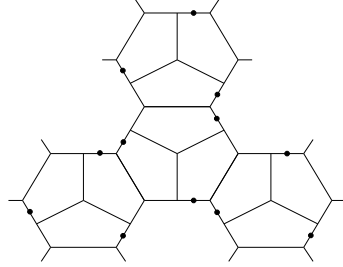


Figure 6.4: An isogonal isohedral  $(6, 4)$ -polycycle



One can consider  $k$ -isotoxal,  $k$ -isohedral and  $k$ -isogonal  $(r, q)$ -polycycles, i.e.,  $(r, q)$ -polycycles with  $k$  orbits of edges, faces, vertices, respectively. The finiteness still holds and the enumeration would still be possible by computer, but the number of possibilities would be much larger and the complexity of the computation is unknown.

Eight families of isohedral  $(r, q)$ -polycycles with  $\text{Aut}(P)$  being a strip group are given in Figure 6.2; all have  $q = 3, 4$ . The points on edges indicate vertices of degree two of depicted polycycles producing those families. We think that there is no other isohedral  $(r, q)$ -polycycles with a strip group.

For any  $r \geq 5$  there exists a continuum of *quasi*-isohedral polycycles, i.e., not isohedral ones, but with all  $r$ -gons having the same corona, i.e., circuit of adjacent faces. In fact, let  $T$  be an infinite, in both directions, path of regular  $r$ -gons, such that for any of them, the edges of adjacency to its neighbors are at distance  $\lfloor \frac{r-3}{2} \rfloor$  and the sequence of (one of two possible) choices of joining each new  $r$ -gon, is aperiodic and different from its reversal. There is a continuum of such paths  $T$  for any  $r \geq 5$ . Any  $T$  is quasi-isohedral and its group of automorphisms is trivial. It is a  $(r, 3)$ -helicene if  $r = 5, 6$  and isometric proper polycycle if  $r \geq 7$ .

### 6.3 Isohedral and isogonal $(r, q)_{\text{gen}}$ -polycycles

The hypothesis of simple connectedness of  $(r, q)$ -polycycle radically simplifies the enumeration of the isohedral and isogonal ones.

Given a  $(r, q)_{\text{gen}}$ -polycycle, which is isohedral, isogonal, then its universal cover is also isohedral, isogonal, respectively. This gives, in principle, a method for enumerating the isohedral, respectively, isogonal  $(r, q)_{\text{gen}}$ -polycycles: enumerate such simple connected ones, i.e., such  $(r, q)$ -polycycles, then take their quotients by adequate groups.

As an illustration, consider the enumeration of isogonal  $(3, 5)_{\text{gen}}$ -polycycles. There are three isogonal  $(3, 5)$ -polycycles: 3-gon,  $APrism_{\infty}$  and the isogonal  $(3, 5)$ -polycycle depicted on Figure 6.3, which we denote by  $P_{3,5}$ . The 3-gon has no possible quotients, the quotients of  $APrism_{\infty}$  are enumerated in Section 4.5. The automorphism group  $\text{Aut}(P_{3,5})$

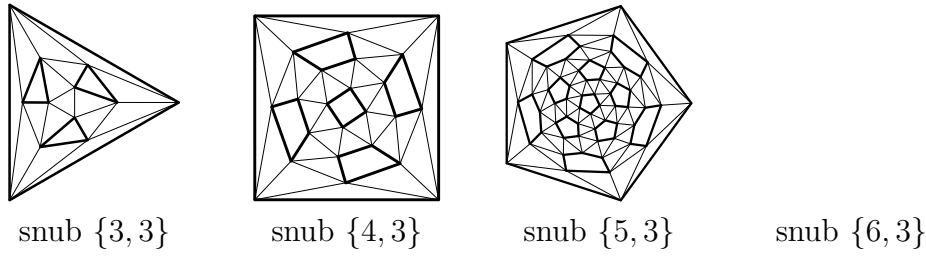


Figure 6.5: Twisted  $\{b, 3\}$  for  $b = 3, 4, 5, 6$

of  $P_{3,5}$  is isomorphic to the modular group  $PSL(2, \mathbb{Z}) \simeq T(2, 3, \infty)$  and the stabilizer of any vertex is trivial.

Let  $G$  be a group of fixed-point-free automorphisms of  $P_{3,5}$  such that the quotient map  $P_{3,5}/G$  is isogonal. Since the group of automorphisms of  $P_{3,5}/G$  is isomorphic to the normalizer  $N_{Aut(P_{3,5})}(G)/G$ , it holds  $N_{Aut(P_{3,5})}(G) = Aut(P_{3,5})$ , since the stabilizer of any vertex is trivial. So,  $G$  has to be a normal subgroup of  $Aut(P_{3,5})$ , in order, for the quotient to be isogonal. There is a large variety of normal fixed-point-free subgroups of  $PSL(2, \mathbb{Z})$  (see [Ne72]) and so, a large variety of isogonal  $(3, 5)_{gen}$ -polycycles.

One class of them, we call them *snub*  $\{b, 3\}$ , is obtained from the regular tiling  $\{b, 3\}$  by replacing every vertex by a 3-gon and every edge by two 3-gons. The snub  $\{b, 3\}$  is a  $(\{3, b\}, 5)$ -map (see Chapter 2). See snub  $\{b, 3\}$  for  $3 \leq b \leq 6$  on Figure 6.5, i.e., some  $(3, 5)_{gen}$ -polycycles with holes being  $b$ -gons. The corona of their vertices is  $3^4.b$ ; so, their skeletons are Icosahedron, Snub Cube, Snub Dodecahedron and Archimedean plane tiling  $(3^4.6)$ , respectively.

# Chapter 7

## Elementary polycycles

We have seen in Section 4.5 a full classification of  $(3,3)_{gen}$ -,  $(3,4)_{gen}$ - and  $(4,3)_{gen}$ -polycycles. We have also seen that, for all other  $(r,q)$ , there is a continuum of  $(r,q)$ -polycycles. The purpose of this chapter is to introduce a decomposition of polycycles into elementary components in an analogous way to decomposition of molecules into atoms. This method will prove to be very effective but only in elliptic case, since, for all other cases, we will show that there is a continuum of such elementary components (see Theorem 7.2.1). First occurrence of the method is in [DeSt02b], followed by [DDS05b] and [DDS05c].

### 7.1 Decomposition of polycycles

Given an integer  $q \geq 3$  and a set  $R \subset \mathbb{N} - \{1\}$  (so, 2-gons will be permitted in this chapter), a  $(R,q)_{gen}$ -polycycle is a non-empty 2-connected map on a surface  $S$  with faces partitioned in two non-empty sets  $F_1$  and  $F_2$ , so that it holds:

- (i) all elements of  $F_1$  (called *proper faces*) are combinatorial  $i$ -gons with  $i \in R$ ;
- (ii) all elements of  $F_2$  (called *holes*, the exterior face(s) are amongst them) are pairwise disjoint, i.e., have no common vertices;
- (iii) all vertices have degree within  $\{2, \dots, q\}$  and all *interior* (i.e., not on the boundary of a hole) vertices are  $q$ -valent.

The map can be finite or infinite and some holes can be  $i$ -gons with  $i \in R$ . If  $R = \{r\}$ , then the above definition corresponds to  $(r,q)_{gen}$ -polycycles. If a  $(R,q)_{gen}$ -polycycle is simply connected, then we call it a  $(R,q)$ -polycycle; those polycycles can be drawn on the plane with the holes being exterior faces.  $(R,q)$ -polycycles with  $R = \{r\}$  are exactly  $(r,q)$ -polycycles considered in Chapters 4–6. An interest of allowing several possible sizes for the interior faces is that aromatic hydrocarbons compounds in Chemistry have a molecular formula, which can modeled on such polycycles, see Figure 7.1. The definition of  $(R,q)$ -polycycles given here is combinatorial; we no longer have the cell-homomorphism into  $\{r,q\}$ . We will define later on elliptic, parabolic, hyperbolic  $(R,q)$ -polycycles but this will no longer have a direct relation to the sign of the curvature of  $\{r,q\}$ .

A *boundary* of a  $(R,q)_{gen}$ -polycycle  $P$  is the boundary of any of its holes.

A *bridge* of a  $(R,q)_{gen}$ -polycycle is an edge, which is not on a boundary and goes from a hole to a hole (possibly, the same). An  $(R,q)_{gen}$ -polycycle is called *elementary* if it has no bridges. See below illustration of those notions:

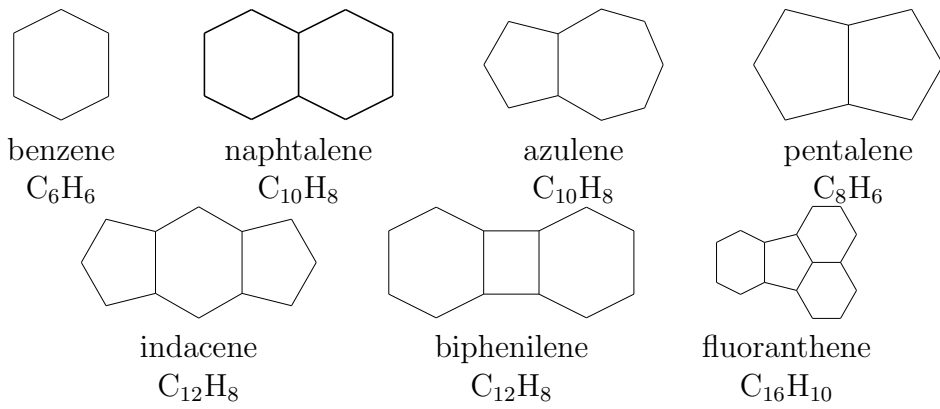
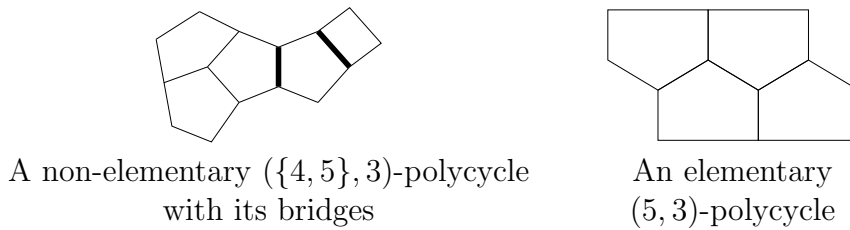


Figure 7.1: Some small aromatic hydrocarbon molecules; here  $C_nH_m$  means  $n$  vertices (carbon atoms) including  $m$  2-valent ones, where a hydrogen atom can be attached (double bonds are omitted for simplicity)



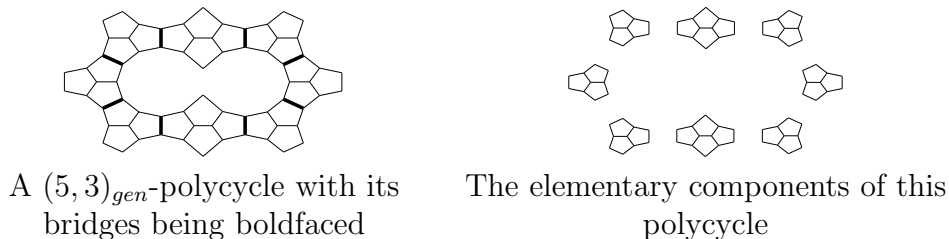
An *open edge* of a  $(R, q)_{gen}$ -polycycle is an edge on a boundary, such that each of its end-vertices have degree less than  $q$ . See below the open edges of some  $(R, q)$ -polycycles:



The open edges of a  $(5, 3)$ -polycycle      The open edge of a  $(\{2, 3\}, 5)$ -polycycle

**Theorem 7.1.1** *Every  $(R, q)_{gen}$ -polycycle is uniquely formed by the agglomeration of elementary  $(R, q)_{gen}$ -polycycles along open edges or, in other words, it can be uniquely cut, along the bridges, into elementary  $(R, q)_{gen}$ -polycycles.*

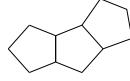
See below an example of such decomposition of a  $(5, 3)_{gen}$ -polycycle on the plane:



Theorem 7.1.1, together with the determination of elliptic elementary  $(r, q)_{gen}$ -polycycles, is used in Chapters 5, 8, 12, 13, 14, 18 for classification purposes.

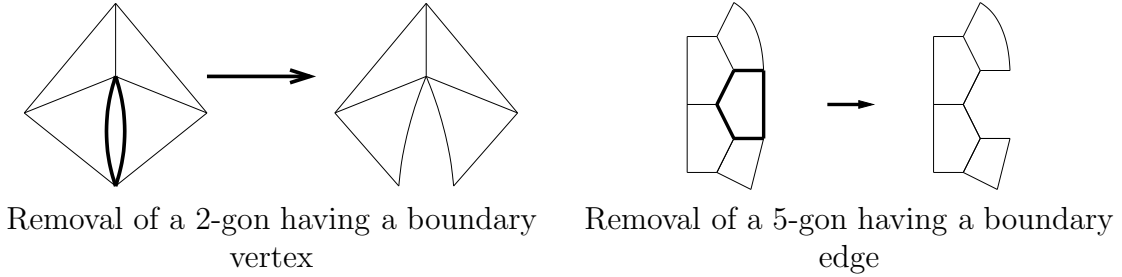
Theorem 7.1.1 gives a simple way to describe an  $(r, q)$ -polycycle: give the names of its elementary components and use the symbol  $+$ . But, in many cases, this is ambiguous,

i.e., the same elementary component can be used to form an  $(r, q)$ -polycycle in different ways, in the same way as the formula of a molecule, giving its number of atoms, does not define it in general. For example, with  $D$  denoting the  $(5, 3)$ -polycycle formed by a 5-gon,  $D + D + D$  refers unambiguously to the following  $(5, 3)$ -polycycle:



There is another  $(5, 3)$ -polycycle with three 5-gons sharing a vertex; it is elementary and named  $E_1$  according to Figure 7.2. But  $D + D + D + D$  is ambiguous, since there are two  $(5, 3)$ -polycycles having four elementary components  $D$ .

Given a  $(R, q)_{gen}$ -polycycle  $P$ , one can define another  $(R, q)_{gen}$ -polycycle  $P'$  by removing a face  $f$  from  $F_1$ , i.e., by considering it as a hole. If  $f$  has no common vertices with other faces from  $F_1$ , then removing it leaves unchanged the plane graph  $G$  and only changes the pair  $(F_1, F_2)$ . If  $f$  has some edges in common with a hole, then we remove them. If  $f$  has a vertex  $v$  in common with a hole and if  $v$  does not belong to a common edge, then we split  $v$  in two vertices. See below two examples of this operation:



The reverse operation is *addition* of a face. A  $(R, q)_{gen}$ -polycycle  $P$  is called *extensible* if there exists another  $(R, q)_{gen}$ -polycycle  $P'$ , such that the removal of a face of  $P'$  yields  $P$ , i.e., if one can add a face to it.

In all pictures below, we put under a  $(R, q)$ -polycycle  $P$ , its symmetry group  $Aut(P)$  and mark *nonext.* for non-extensible  $P$  (see Section 8.2 for details on this notion). Also, we put in parenthesis the group  $Aut(G)$  of the plane graph  $G$  of  $P$  if  $Aut(P) \neq Aut(G)$  and no other polycycle with the same plane graph exists. Our setting here is more general than in Chapter 4; the plane graph no longer determines the polycyclic realization. In fact, the same plane graph  $G$  can admit several realizations as a  $(R, q)$ -polycycle; see examples in Appendices 1 and 2.

A natural question is, if one can further enlarge the class of polycycles.

There will be only some technical difficulties if one try to obtain the catalog of elementary  $(R, Q)$ -polycycles, i.e., the generalization of  $(R, q)$ -polycycles allowing the set  $Q$  for values of degree of interior vertices. Such polycycle is called *elliptic*, *parabolic* or *hyperbolic* if  $\frac{1}{q} + \frac{1}{r} - \frac{1}{2}$  (where  $r = \max_{i \in R} i$ ,  $q = \max_{i \in Q} i$ ) is positive, zero or negative, respectively. The decomposition and other main notions could be applied directly.

We required 2-connectedness and that any two holes do not share a vertex. If one removes those two hypothesis, then many other graphs do appear.

The omitted cases  $(R, q) = (2, q)$  are not interesting. In fact, consider infinite series of  $(2, 6)$ -polycycles, tripled  $m$ -gons,  $m \geq 2$  (i.e.,  $m$ -gon with each edge being tripled). The central edge is a bridge for those polycycles, for both 2-gons of the triple of edges. But if one removes those two 2-gons, then the resulting plane graph has two holes sharing a face, i.e., violates the crucial point (ii) of the definition of  $(R, q)$ -polycycle. For even  $m$ ,

each even edge (for some order  $1, \dots, m$  of them) can be duplicated  $t$  times (for fixed  $t$ ,  $1 \leq t \leq 5$ ), and each odd edge duplicated  $6 - t$  times; so, the degrees of all vertices will be still 6. On the other hand, two holes ( $m$ -gons inside and outside of the tripled  $m$ -gon) have common vertices; so, it is again not our polycycle.

## 7.2 Parabolic and hyperbolic elementary $(R, q)_{gen}$ -polycycles

The interesting question is to enumerate, if possible, those elementary  $(R, q)_{gen}$ -polycycles. Call a  $(R, q)_{gen}$ -polycycle *elliptic*, *parabolic* or *hyperbolic* if the number  $\frac{1}{r} + \frac{1}{q} - \frac{1}{2}$  (where  $r = \max_{i \in R} i$ ) is positive, zero or negative, respectively. In Theorem 7.2.1, we will see that the number of elementary  $(r, q)$ -polycycles is uncountable for any parabolic or hyperbolic pairs  $(r, q)$ . But in [DeSt01] and [DeSt02b], all elliptic elementary  $(r, q)$ -polycycles were determined. See Figures 7.2 and 7.3 for the list of elementary  $(5, 3)$ - and  $(3, 5)$ -polycycles, which will be needed later. For  $(3, 3)$ -,  $(3, 4)$ - and  $(4, 3)$ -polycycles, we have full classification of them in Chapter 4. In fact, we will consider the case  $R = \{i : 2 \leq i \leq r\}$  covering all elliptic possibilities:  $(\{2, 3, 4, 5\}, 3)$ -,  $(\{2, 3\}, 4)$ - and  $(\{2, 3\}, 5)$ -polycycles in Sections 7.4, 7.5 and 7.6, respectively. Call *kernel* of a polycycle, the cell-complex of its vertices, edges and faces, which are not incident with its boundary.

**Theorem 7.2.1** *For parabolic and hyperbolic parameters  $(r, q)$ , there exists a continuum of non-isomorphic elementary  $(r, q)$ -polycycles.*

**Proof.** Consider a semi-infinite (to the right) chain of 4-gons that fill a strip between two parallel rays. Inside two horizontal sides of each 4-gon of the chain, we put  $r - 5$  and one new vertices to obtain an  $r$ -gon instead of a 4-gon. There are two alternatives: either  $r - 5$  new vertices are placed on the upper side and one on the lower side or vice versa, one new vertex is placed on the upper side and  $r - 5$  on the lower. Such a choice is made independently on each 4-gon when we move to the right along this chain. Therefore, there is a continuum of various (non-isomorphic) chains of this kind. All of them are chains in the tiling  $\{r, q\}$  for  $r \geq 7$  and  $q \geq 3$ , as well as for  $r = 5$  and  $q \geq 4$ . It is also clear that this  $(r, q)$ -polycycle is the kernel of an elementary  $(r, q)$ -polycycle consisting of this polycycle supplemented with all  $r$ -gons that are incident to it in the tiling  $\{r, q\}$ .

Now, consider the case of parabolic parameters  $(r, q)$ , i.e.,  $(r, q) = (6, 3)$ ,  $(4, 4)$ , and  $(3, 6)$ . In the square lattice, i.e., in the regular tiling  $\{4, 4\}$  of the Euclidean plane  $\mathbb{R}^2$ , we construct a chain of 4-gons semi-infinite in the upper right direction. On each step of this construction, there are two alternatives for choosing the next 4-gon: one can choose an adjacent 4-gon, either on the right on the same level, or one level higher. It is clear that there is a continuum of various (non-isomorphic) chains of this kind in the tiling  $\{4, 4\}$  and each of these chains is the kernel of a certain elementary  $(4, 4)$ -polycycle. Infinite chains of hexagons in the tiling  $\{6, 3\}$  are constructed analogously. As for the tiling  $\{3, 6\}$ , combining two adjacent 3-gons in it into a rhomb and transforming the entire tiling  $\{3, 6\}$  into a rhombic lattice combinatorially equivalent to the tiling  $\{4, 4\}$ , one can apply the same line of reasoning as in the case of the square lattice. The kernels of those parabolic polycycles are outerplanar. They can be interpreted as the kernels of hyperbolic polycycles (by increasing the value of the parameter  $q$ ).  $\square$

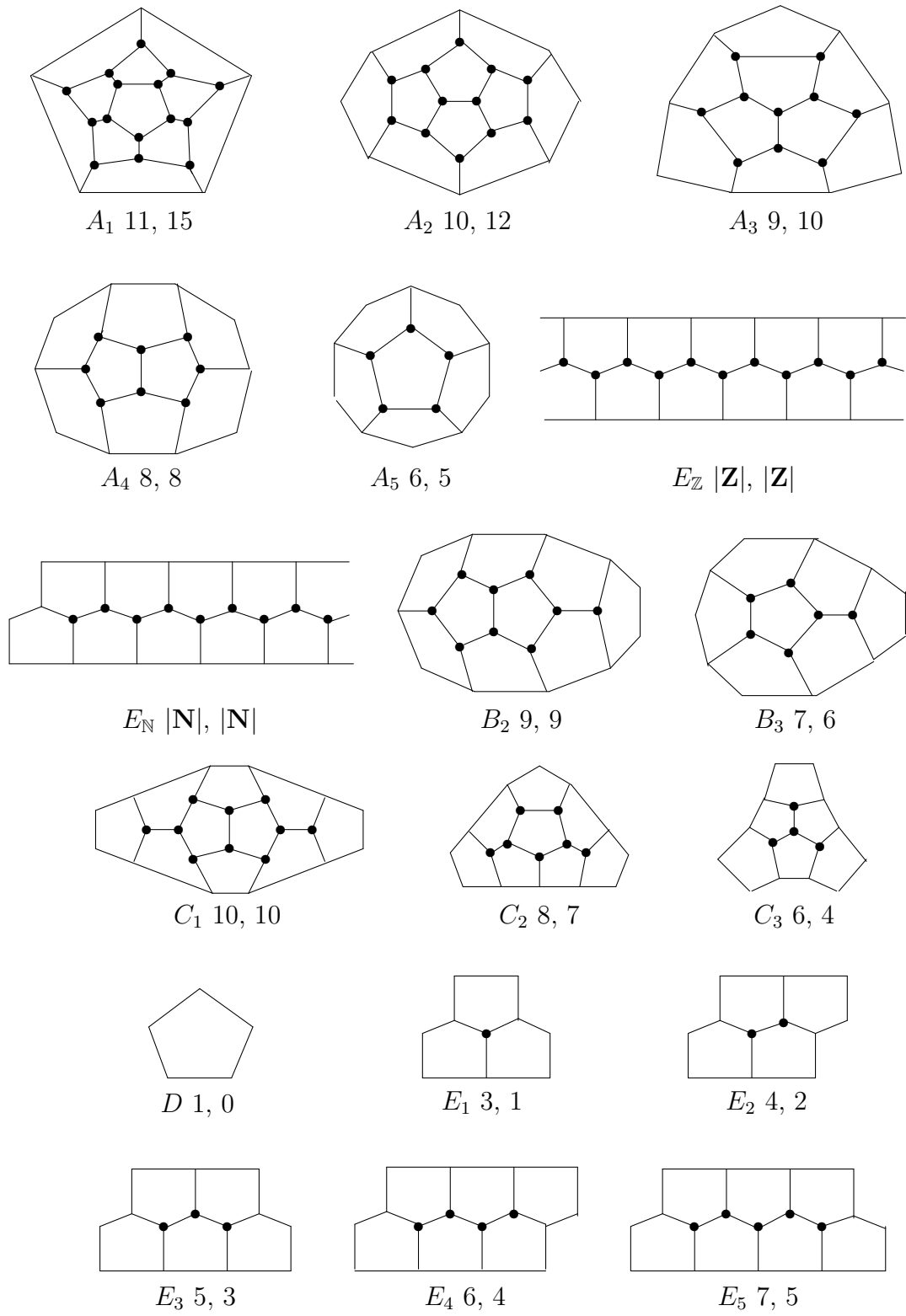


Figure 7.2: Elementary (5,3)-polycycles and their kernels

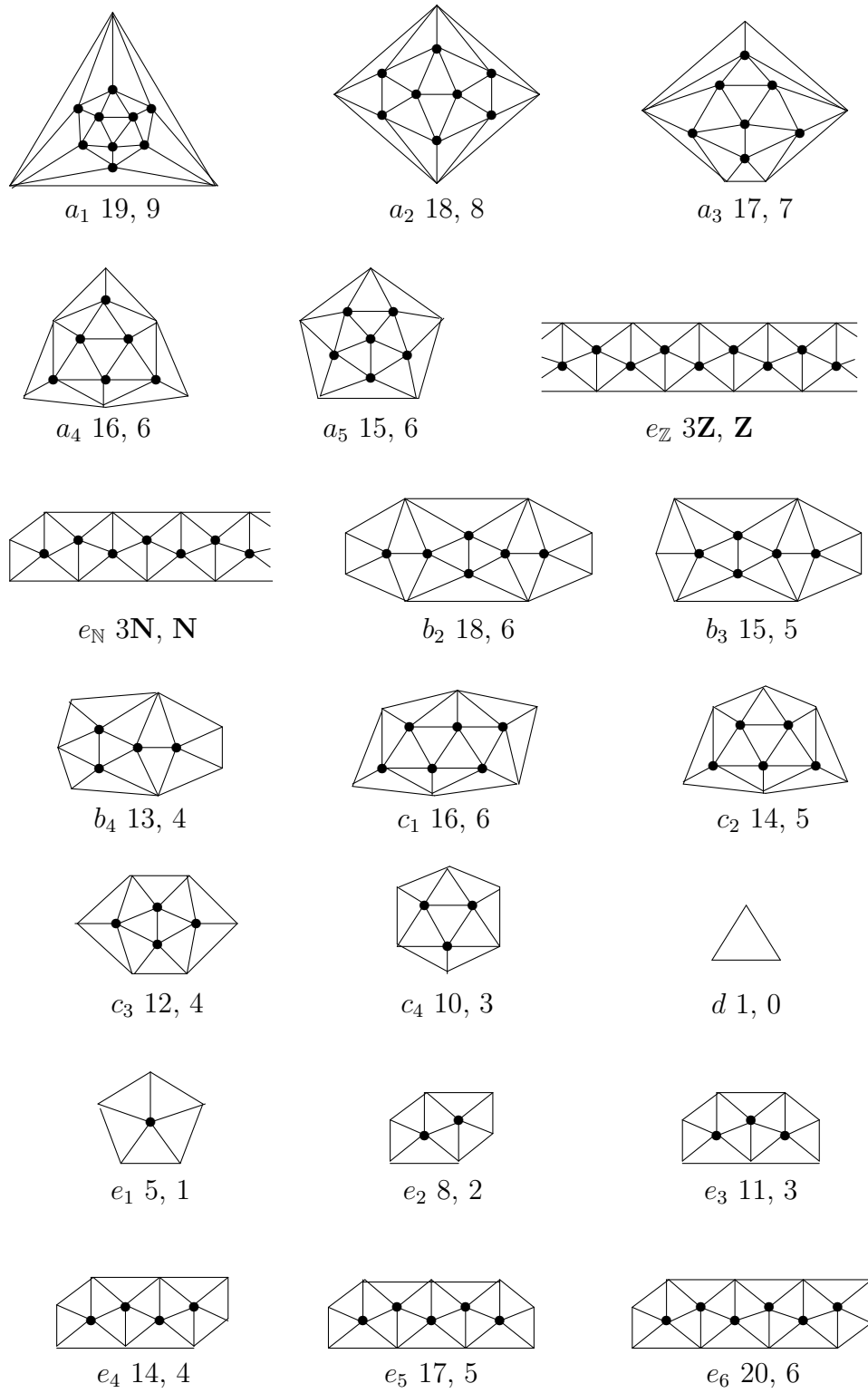


Figure 7.3: Elementary (3, 5)-polycycles and their kernels

## 7.3 Kernel-elementary polycycles

Call a  $(r, q)$ -polycycle *kernel-elementary* if it is an  $r$ -gon or if it has non-empty connected kernel, such that the deletion of any face from the kernel will diminish it (i.e., any face of the polycycle is incident to its kernel).

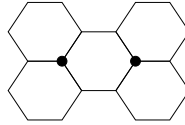
**Theorem 7.3.1** (i) *If a  $(r, q)$ -polycycle is kernel-elementary, then it is elementary.*

(ii) *If  $(r, q)$  is elliptic then any elementary  $(r, q)$ -polycycle is also kernel-elementary.*

**Proof.** (i) Take a kernel-elementary  $(r, q)$ -polycycle  $P$ ; one can assume it to be different from an  $r$ -gon. Let  $P_1, \dots, P_r$  be the elementary components of this polycycle. The connectedness condition on the kernel gives that all  $P_i$  but one are  $r$ -gons. But removing the  $r$ -gonal  $P_i$  does not change the kernel; so,  $P$  is elementary.

(ii) Consider any two vertices of an  $r$ -gon of an elliptic  $(r, q)$ -polycycle that belongs to the kernel of this polycycle. The shortest edge path between these vertices lies inside the union of two stars of  $r$ -gons with the centers at these two vertices; this result can easily be verified in each particular case for any elliptic parameters  $(r, q) = (3, 3), (3, 4), (3, 5), (4, 3)$  and  $(5, 3)$ . Hence, any  $r$ -gon of an elliptic  $(r, q)$ -polycycle is only incident with one simply connected component of its kernel. All  $r$ -gons that are incident with the same non-empty connected component of the kernel constitute a non-trivial elementary summand. Since the polycycle is elementary, this is its totality and the kernel is connected.  $\square$

In [DeSt02b] the notion of kernel-elementary was called *elementary*. See below an example of a  $(6, 3)$ -polycycle, which is elementary but not kernel-elementary (since its kernel is not connected):



The decomposition Theorem 7.1.1 (of  $(r, q)$ -polycycles into elementary polycycles) is the main reason why we prefer property to be elementary to kernel-elementary one. Another reason is that if a  $(r, q)_{gen}$ -polycycle is elementary, then its universal cover is also elementary. However, the notion of kernel elementariness will be useful in the classification of infinite elementary  $(\{3, 4, 5\}, 3)$ - and  $(\{2, 3\}, 5)$ -polycycles.

In Figures 7.2 and 7.3, each elementary polycycle is denoted by a certain letter with a subscript; two numbers indicate the values of the parameters  $p_r$  (the number of interior faces) and  $v_{int}$  (the number of interior vertices). The infinite series  $E_s$ , respectively  $e_s$  have  $(p_r, v_{int}) = (s + 2, s)$ , respectively  $(3s + 2, s)$  and are represented for  $s \leq 5$ , respectively  $s \leq 6$ .

**Theorem 7.3.2** *The list of elementary  $(5, 3)$ -polycycles (see Figure 7.2) consists of:*

- (i) 11 sporadic finite  $(5, 3)$ -polycycles,
- (ii) an infinite series  $E_n$ ,  $n \geq 1$ ,
- (iii) two infinite polycycles  $E_{\mathbb{N}}$  and  $E_{\mathbb{Z}}$  (snub  $Prism_{\infty}$ ).

**Proof.** Take an elementary  $(5, 3)$ -polycycle  $P$  which, by Theorem 7.3.1, is kernel-elementary. If its kernel is empty, then  $P$  is simply  $D$ . If the kernel is reduced to a vertex, then  $P$  is simply  $E_1$ . If each 5-gon of an elementary  $(5, 3)$ -polycycle has at most three vertices from the kernel, that are arranged in succession along the perimeter of the 5-gon, then the kernel does not contain 5-gons and has the form of a *geodesic* (see the elementary  $(5, 3)$ -polycycles  $E_i$ ,  $i \geq 1$ ,  $E_{\mathbb{N}}$ , and  $E_{\mathbb{Z}}$ ) or a *propeller* (see the elementary  $(5, 3)$ -polycycle  $C_3$ ). If at least one 5-gon of the elementary  $(5, 3)$ -polycycle contains three vertices of the kernel that are arranged along the perimeter not in succession, then the whole 5-gon belongs to the kernel. Only in the case of one or two 5-gons, the kernel can additionally contain one or two pendant edges (see  $(5, 3)$ -polycycles  $A_5$ ,  $B_3$ ,  $C_2$  and  $A_4$ ,  $B_2$ ,  $C_1$ ). If the kernel contains more than two 5-gons, then the total number of these 5-gons can only be 3, 4, or 6 (see  $A_3$ ,  $A_2$ , and  $A_1$ ).  $\square$

**Theorem 7.3.3** *The list of elementary  $(3, 5)$ -polycycles (see Figure 7.3) consists of:*

- (i) 13 sporadic finite  $(3, 5)$ -polycycles,
- (ii) an infinite series  $e_n$ ,  $n \geq 1$ ,
- (iii) two infinite polycycles  $e_{\mathbb{N}}$  and  $e_{\mathbb{Z}}$  (snub  $APrism_{\infty}$ ).

**Proof.** Take an elementary  $(3, 5)$ -polycycle  $P$  which, by Proposition 7.3.1, is kernel-elementary. If its kernel is empty, then  $P$  is simply  $d$ . If the kernel is reduced to a vertex, then  $P$  is simply  $e_1$ . If there are at most two vertices from a kernel in each 3-gon, then the kernel does not contain 3-gons and has the form of a *geodesic* (see  $e_i$ ,  $i \geq 1$ , as well as  $e_{\mathbb{N}}$  and  $e_{\mathbb{Z}}$ ). If there is one 3-gon in a kernel, the latter may additionally have one pendant edge (see  $c_4$  and  $b_4$ ). If there are two 3-gons in a kernel, the latter may additionally have one or two pendant edges (see  $c_3$ ,  $b_3$ , and  $b_2$ ). If there are more than two 3-gons in a kernel, then their total number may only be 3, 4, 5, 6, 8, or 10 (see  $a_1$ ,  $a_2$ ,  $a_3$ ,  $a_4$ ,  $a_5$ ,  $c_1$ , and  $c_2$ ).  $\square$

Remark that the kernels of  $(5, 3)$ -polycycles  $A_i$ ,  $1 \leq i \leq 5$ , of Figure 7.2 are all non-trivial isometric subgraphs  $(5, 3)$ -polycycles; they are also all *circumscribed*  $(5, 3)$ -polycycles, i.e.,  $r$ -gons can be added around the perimeter, so that they will form a simple circuit. (They were found in [CCBBZGT93]; such  $(5, 3)$ -polycycles are useful in Organic Chemistry.) All circumscribed  $(3, 5)$ -polycycles are the kernels of polycycles  $a_i$ ,  $1 \leq i \leq 5$ , and  $c_i$ ,  $1 \leq i \leq 4$  of Figure 7.3. It turns out that all polycycles  $P$  in one of Figures 7.2 and 7.3, admitting the inner dual polycycle  $Inn^*(P)$  in another one, are as follows:

|                    |                    |                    |                    |
|--------------------|--------------------|--------------------|--------------------|
| $Inn^*(A_1) = a_5$ | $Inn^*(A_2) = c_3$ | $Inn^*(A_3) = c_4$ | $Inn^*(A_4) = e_2$ |
| $Inn^*(A_5) = e_1$ | $Inn^*(E_1) = d$   | $Inn^*(a_1) = A_3$ | $Inn^*(a_2) = A_4$ |
| $Inn^*(a_4) = C_3$ | $Inn^*(a_5) = A_5$ | $Inn^*(c_1) = E_4$ | $Inn^*(c_2) = E_3$ |
| $Inn^*(c_3) = E_2$ | $Inn^*(c_4) = E_1$ | $Inn^*(e_1) = D$   |                    |

$E_{\mathbb{Z}}$ =snub  $Prism_{\infty}$  occurs also in Figure 6.1; its inner dual is infinite  $(3, 4)$ -polycycle  $APrism_{\infty}$ .

**Theorem 7.3.4** *All elementary  $(5, 3)_{gen}$ -polycycles, which are not  $(5, 3)$ -polycycles, are:*

- (i) the plane graphs snub  $Prism_m$  with two holes (both  $m$ -gonal faces removed), for any  $m \geq 2$ ,

- (ii) the (non-orientable, on Möbius surface) quotient of snub  $Prism_m$ , for any odd  $m$ , with respect to central symmetry.

**Proof.** Take such a polycycle. Its universal cover is an elementary  $(5, 3)$ -polycycle, whose group of automorphism contains some fixed-point-free transformation. Inspection of the list of elementary  $(5, 3)$ -polycycles on Figure 7.2 yields only  $E_{\mathbb{Z}} = \text{snub } Prism_{\infty}$  as a possibility. Snub  $Prism_m$  is obtained from the group of translations by  $m$  faces and the non-orientable quotients if the group contains also some translation followed by symmetry.  $\square$

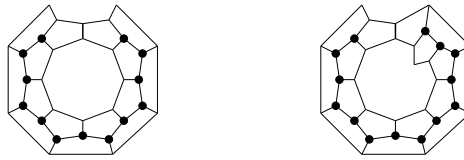
**Theorem 7.3.5** *All elementary  $(3, 5)_{gen}$ -polycycles, which are not  $(3, 5)$ -polycycles, are:*

- (i) the plane graphs snub  $APrism_m$  with two holes (both  $m$ -gonal faces removed), for any  $m \geq 2$ ,
- (ii) the (non-orientable, on Möbius surface) quotient of snub  $APrism_m$  for any odd  $m$ , with respect to central symmetry.

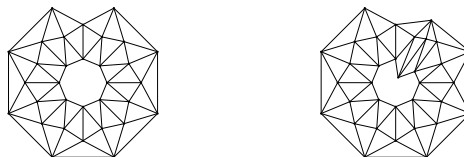
**Proof.** Take such a polycycle. Its universal cover is an elementary  $(3, 5)$ -polycycle, whose group of automorphisms contains some fixed-point-free transformation. Inspection of the list of elementary  $(3, 5)$ -polycycles on Figure 7.3 yields only  $e_{\mathbb{Z}} = \text{snub } APrism_{\infty}$  as possibility. The arguments follow as before.  $\square$

We can now classify all kernel-elementary elliptic  $(r, q)_{gen}$ -polycycles obtained in [DDS05b]. Such a polycycle is either elementary, or it is obtained by self-gluing of an elementary  $(r, q)$ -polycycle. Hence, the list is as follows:

1. All kernel-elementary  $(5, 3)_{gen}$  polycycles, obtained by self-gluing of elementary  $(5, 3)$ -polycycles, are  $E_{n,or}^*$ ,  $E_{n,nor}^*$ ,  $C_{1,or}^*$ ,  $C_{1,nor}^*$ ,  $C_{2,or}^*$ ,  $C_{2,nor}^*$ ,  $C_{3,or}^*$ ,  $C_{3,nor}^*$ . The symbol  $*$  refer to the self-gluing and subscripts *or*, *nor* are used if the self-gluing is orientable or not, respectively. See below  $E_{13,or}^*$  and  $E_{14,or}^*$ :



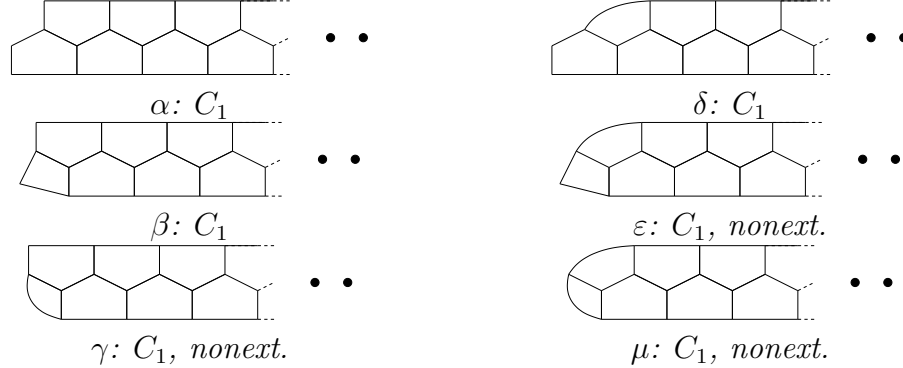
2. All kernel-elementary  $(5, 3)_{gen}$  polycycles, obtained by self-gluing of elementary  $(5, 3)$ -polycycles are  $e_{n,or}^*$ ,  $e_{n,nor}^*$ ,  $b_{2,or}^*$ ,  $b_{2,nor}^*$ . The symbols  $*$ , *or*, *nor* are used as above. See below  $e_{15,or}^*$  and  $e_{16,or}^*$ :



## 7.4 Classification of elementary $(\{2, 3, 4, 5\}, 3)_{\text{gen}}$ -polycycles

**Theorem 7.4.1** *The list of elementary  $(\{2, 3, 4, 5\}, 3)_{\text{gen}}$ -polycycles consists of:*

- (i) 204 sporadic  $(\{2, 3, 4, 5\}, 3)$ -polycycles given in Appendix 1.
- (ii) Six  $(\{3, 4, 5\}, 3)$ -polycycles, infinite in one direction:



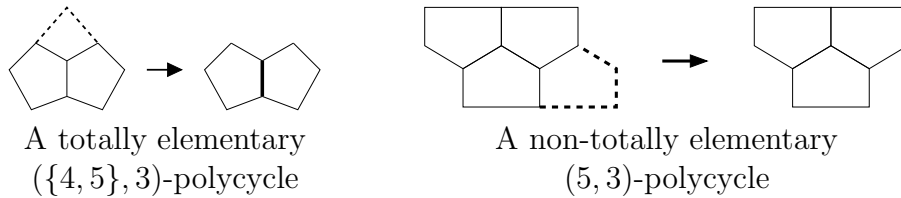
- (iii)  $21 = \binom{6+1}{2}$  infinite series obtained by taking two endings of the infinite polycycles of (ii) above and concatenating them.

For example, merging of  $\alpha$  with itself produces the infinite series of elementary  $(5, 3)$ -polycycles, denoted on Figure 7.2 by  $E_n$ ,  $0 \leq n \leq \infty$ . See Figure 7.4 for the first 3 members (starting with 6 faces) of two such series:  $\alpha\alpha$  and  $\beta\epsilon$ .

- (iv) The infinite series of snub  $\text{Prism}_m$ ,  $2 \leq m \leq \infty$ , and its non-orientable quotient for  $n$  odd.

**Proof.** The first step is to determine all elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles, which contain a 2-gon. This is done in Lemma 7.4.2. So, in the following, we consider only elementary  $(\{3, 4, 5\}, 3)$ -polycycles.

A  $(R, 3)$ -polycycle is called *totally elementary* if it is elementary and if, after removing any face adjacent to a hole, one obtains a non-elementary  $(R, 3)$ -polycycle. So, an elementary  $(R, 3)$ -polycycle is totally elementary if and only if it is not the result of an extension of some elementary  $(R, 3)$ -polycycle. See below an illustration of this notion:

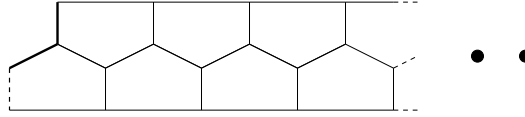


All totally elementary  $(\{3, 4, 5\}, 3)$ -polycycles are enumerated in Lemma 7.4.3. We will now classify all finite elementary  $(\{3, 4, 5\}, 3)$ -polycycles with one hole. Such a polycycle with  $N$  interior faces is either totally elementary, or it is obtained from another such polycycle with  $N - 1$  interior faces by addition of a face. There is no elementary  $(\{3, 4, 5\}, 3)$ -polycycles with 2 interior faces; so, all elementary  $(\{3, 4, 5\}, 3)$ -polycycles with 3 interior faces are totally elementary and, by Lemma 7.4.3, we know them. Also, by Lemma 7.4.3, there are no finite totally elementary  $(\{3, 4, 5\}, 3)$ -polycycles with more than 3 interior faces. We iterate the following procedure starting at  $N = 3$ :

1. Take the list of finite elementary  $(\{3, 4, 5\}, 3)$ -polycycles with  $N$  interior faces and add a face in all possible ways, while preserving the property to be an elementary  $(\{3, 4, 5\}, 3)$ -polycycle.
2. Reduce by isomorphism and obtain the list of elementary  $(\{3, 4, 5\}, 3)$ -polycycles with  $N + 1$  interior faces.

So, for any fixed  $N$ , one obtains the list of elementary  $(\{3, 4, 5\}, 3)$ -polycycles with  $N$  interior faces. The enumeration is done in the following way: run the computation up to  $N = 13$  and obtain the sporadic elementary  $(\{3, 4, 5\}, 3)$ -polycycles and the members of the infinite series. Then do, by hand, the operation of addition of a face and reduction by isomorphism; one obtains only the 21 infinite series for all  $N \geq 13$ . This complete the enumeration of finite elementary  $(\{3, 4, 5\}, 3)$ -polycycles.

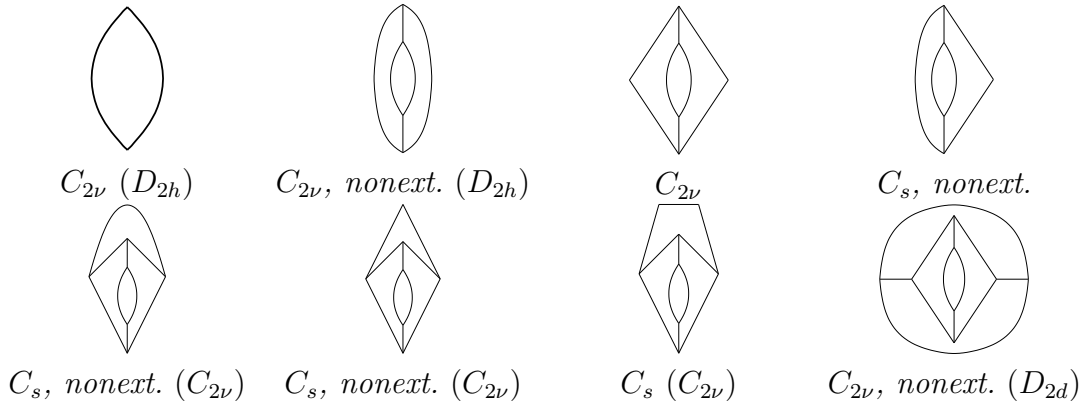
Take now an elementary infinite  $(\{3, 4, 5\}, 3)$ -polycycle  $P$ . Remove all 3- or 4-gonal faces of it. The resulting graph  $P'$  is not necessarily connected, but its connected components are  $(5, 3)_{gen}$ -polycycles, though not necessarily elementary ones. We will now use the classification of elementary  $(5, 3)_{gen}$ -polycycles (possibly, infinite) done in Theorem 7.3.2. If the infinite  $(5, 3)$ -polycycle snub  $Prism_\infty$  appears in the decomposition, then, clearly,  $P$  is reduced to it. If the infinite polycycle  $\alpha = E_{\mathbb{N}}$  appears in the decomposition, then there are two possibilities for extending it, indicated below:



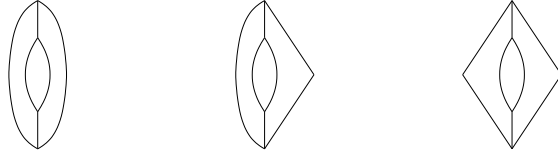
If a 3- or 4-gonal face is adjacent on the dotted line, then there should be another face on the boldfaced edges. So, in any case, there is a face, adjacent on the boldfaced edges, and we can assume that it is a 3- or 4-gonal face. Then, consideration of all possibilities to extend it, yields  $\beta, \dots, \mu$ . Suppose now, that  $P'$  does not contain any infinite  $(5, 3)_{gen}$ -polycycles. Then we can find an infinite path  $f_0, \dots, f_i, \dots$  of distinct faces of  $P$  in  $F_1$ , the set of proper face, such that  $f_i$  is adjacent to  $f_{i+1}$  and  $f_{i-1}$  is not adjacent to  $f_{i+1}$ . The condition on  $P$  implies that an infinite number of faces are 3- or 4-gons, but the condition of non-adjacency of  $f_{i-1}$  with  $f_{i+1}$  forbids 3-gons. Take now a 4-gon  $f_i$  and assume that  $f_{i-1}$  and  $f_{i+1}$  are 5-gons. The consideration of all possibilities of extension around that face, leads us to an impossibility. If some of  $f_{i-1}$  or  $f_{i+1}$  are 4-gons, then we have a path of 4-gons and the case is even simpler.

Let us now determine all elementary  $(\{2, 3, 4, 5\}, 3)_{gen}$ -polycycles. The universal cover  $\tilde{P}$  of such a polycycle  $P$  is an elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycle, which has a non-trivial fixed-point-free automorphism group in  $Aut(\tilde{P})$ . Consideration of the above list of polycycles yields snub  $Prism_\infty$  as the only possibility. The polycycles snub  $Prism_m$  and its non-orientable quotients arise in this process.  $\square$

**Lemma 7.4.2** *All elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles, containing a 2-gon, are the following eight ones:*



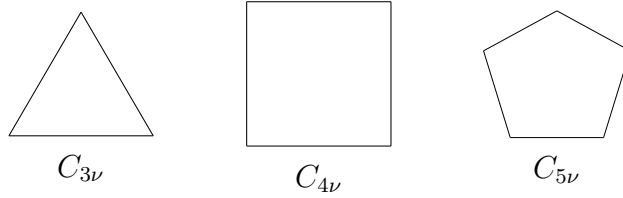
**Proof.** Let  $P$  be such a polycycle. Clearly, the 2-gon is the only possibility if the number of proper  $|F_1|$  is 1. If  $|F_1| = 2$ , then it is not elementary. If  $|F_1| \geq 3$ , then the 2-gon should be inside of the structure. So,  $P$  contains, as a subgraph, one of three following graphs:



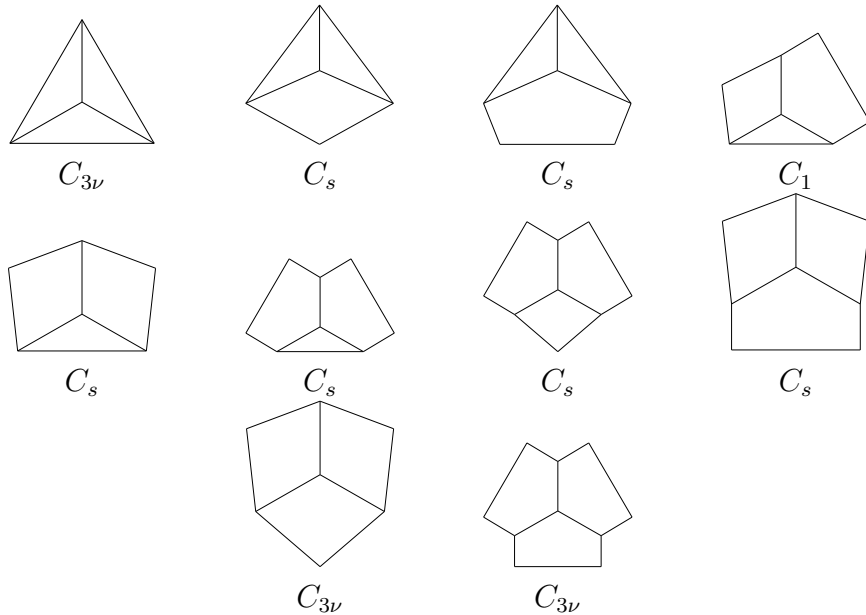
Therefore, the only possibilities for  $P$  are those given in above lemma.  $\square$

**Lemma 7.4.3** *The list of totally elementary  $(\{3, 4, 5\}, 3)$ -polycycles consists of:*

(i) *Three isolated  $i$ -gons,  $i \in \{3, 4, 5\}$ :*



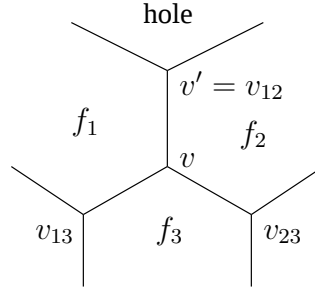
(ii) *Ten triples of  $i$ -gons,  $i \in \{3, 4, 5\}$ :*



(iii) *snub Prism*<sub>∞</sub>.

**Proof.** Take a totally elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycle  $P$ . If  $|F_1| = 1$ , then  $P$  is, clearly, totally elementary; so, let us assume that  $|F_1| \geq 2$ . If  $|F_1| = 2$ , then it is, clearly, not elementary; so, assume  $|F_1| \geq 3$ . Of course,  $P$  has at least one interior vertex; let  $v$  be such a vertex. Furthermore, one can assume that  $v$  is adjacent to a vertex  $v'$ , which is incident to a hole.

The vertex  $v$  is incident to three faces  $f_1, f_2, f_3$ . Let us denote by  $v_{ij}$  unique vertex incident to  $f_i, f_j$  and adjacent to  $v$ . Without loss of generality, one can suppose that  $v'$  is incident to the faces  $f_1$  and  $f_2$ , i.e., that  $v' = v_{12}$ .



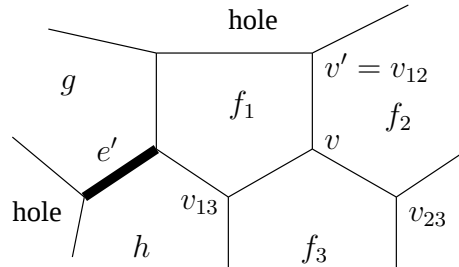
The removal of the face  $f_1$  yields a non-elementary polycycle; so, there is at least one bridge separating  $P - f_1$  in two parts. Such bridge should have an end-vertex incident to  $f_1$ . The same holds for  $f_2$ . The proof consists of a number of cases.

**1<sup>st</sup> case:** If  $e_1 = \{v, v_{23}\}$  and  $e_2 = \{v, v_{13}\}$  are bridges for  $P - f_1, P - f_2$ , respectively, then from the constraint that faces  $f_i$  are  $p$ -gons with  $p \leq 5$ , one sees that each face  $f_i$  is adjacent in  $P$  to at most one other face. Furthermore, if  $f_i$  is adjacent to another face, then this adjacency is along a bridge, which is forbidden. Hence,  $F_1 = \{f_1, f_2, f_3\}$ .

**2<sup>nd</sup> case:** Let us assume now that  $e_1 = \{v, v_{23}\}$  is a bridge for  $P - f_1$ , but  $e_2 = \{v, v_{13}\}$  is not a bridge for  $P - f_2$ . Then, since  $f_2$  is a  $p$ -gon with  $p \leq 5$ , it is adjacent to at most one other face and, if so, then along a bridge, which is impossible. So,  $f_2$  is adjacent to only  $f_1$  and  $f_3$  and, since  $e_2$  is not a bridge for  $P - f_2$ , one obtains that  $P - f_2$  is elementary, which contradicts the hypothesis.

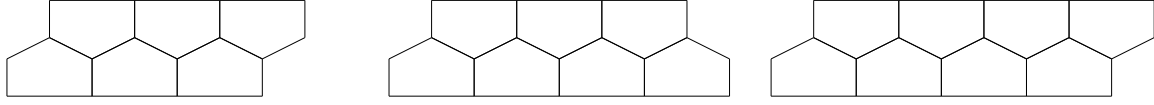
**3<sup>rd</sup> case:** Let us assume that neither  $e_1$ , nor  $e_2$  are bridges for  $P - f_1$  and  $P - f_2$ . From the consideration of previous two cases, one has that every vertex  $v$ , adjacent to a vertex on the boundary, is in this 3<sup>rd</sup> case.

The first subcase, which can happen only if  $f_1$  is 5-gon, happens when the boldfaced edge  $e'$ , in the drawing below, is a bridge.



The face  $g$  is adjacent to the faces  $h$  and  $f_1$  and, possibly, to another face  $g'$ . But if  $g$  is adjacent to such a face  $g'$ , it is along a bridge of  $P$ ; hence,  $g$  is adjacent only to  $h$  and  $f_1$ . So,  $P - g$  is elementary, which is impossible.

Infinite series  $\alpha\alpha$  of elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles ( $E_4$ - $E_6$ ):



Infinite series  $\beta\varepsilon$  of elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles:

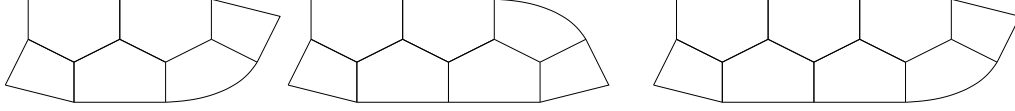
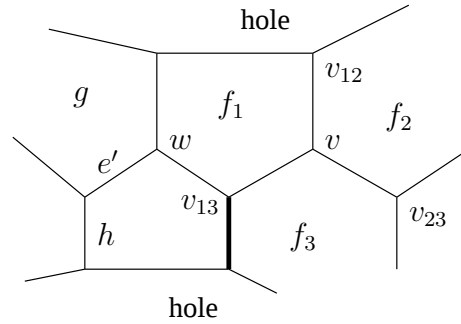


Figure 7.4: The first 3 members (starting with 6 faces) of two infinite series, amongst 21 series of  $(\{2, 3, 4, 5\}, 3)$ -polycycles in Theorem 7.4.1 (v)

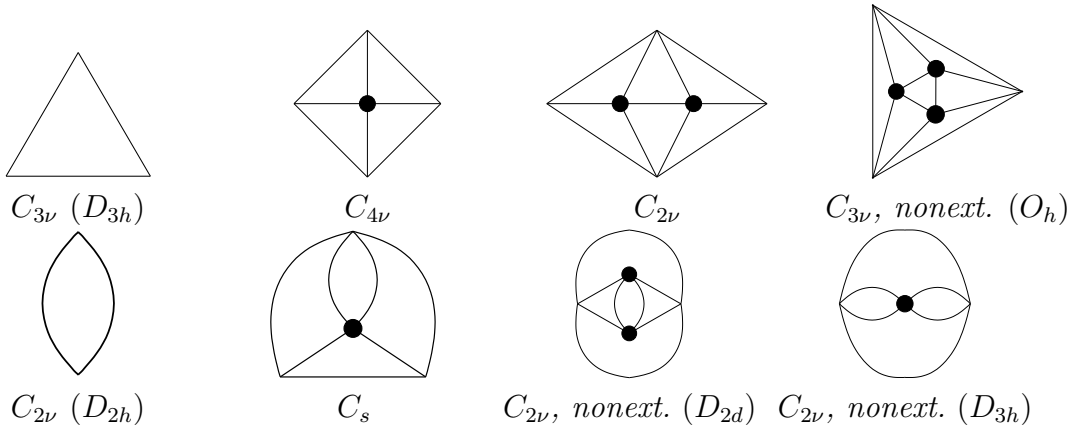
So, the edge  $e'$  is not a bridge and this forces the face  $h$  to be 5-gonal. Hence, the vertex  $v_{13}$  is in the same situation as the vertex  $v$ , described in the diagram below:



So, one can repeat the construction. If, at some point,  $e_1$  is a bridge, then the construction stops; otherwise, one can continue indefinitely and obtains snub  $Prism_\infty$ .  $\square$

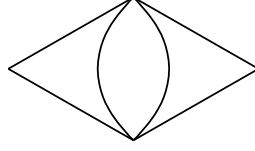
## 7.5 Classification of elementary $(\{2, 3\}, 4)_{gen}$ -polycycles

**Theorem 7.5.1** *Any elementary  $(\{2, 3\}, 4)_{gen}$ -polycycle is one of the following eight:*



**Proof.** The list of elementary  $(3, 4)$ -polycycles is determined by inspecting the list in Section 4.2 and consists of the first four graphs of this theorem. Let  $P$  be a  $(\{2, 3\}, 4)$ -polycycle, containing a 2-gon. If  $|F_1| = 1$ , then it is the 2-gon. Clearly, the case, in which

two 2-gons share one edge, is impossible. Assume that  $P$  contains two 2-gons, which share a vertex. Then we should add 3-gons on both sides and so, obtain the eighth above polycycle. If there is a 2-gon, which does not share a vertex with a 2-gon, then  $P$  contains the following pattern:



So, clearly,  $P$  is fifth or sixth possibility above.  $\square$

Note that seventh and fourth polycycles in Theorem 7.5.1 are, respectively,  $APrism_2$  and  $APrism_3$ ; here the exterior face is the unique hole.

## 7.6 Classification of elementary $(\{2, 3\}, 5)_{gen}$ -polycycles

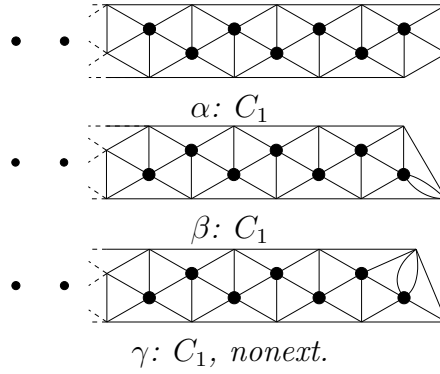
Let us consider an elementary  $(\{2, 3\}, 5)$ -polycycle  $P$ . Assume that  $P$  is not an  $i$ -gon and has a 2-gonal face  $f$ . If  $f$  is adjacent to a hole, then the polycycle is not elementary. So, holes are adjacent only to 3-gons. If one removes such a 3-gon  $t$ , then the third vertex  $v$  of  $t$ , which is necessarily interior in  $P$ , becomes non-interior in  $P - t$ . The polycycle  $P - t$  is not necessarily elementary. Let us denote by  $e_1, \dots, e_5$  the edges incident to  $v$  and assume that  $e_1, e_2$  are edges of  $t$ . The boundary is adjacent only to 3-gons. The potential bridges in  $P - t$  are  $e_3, e_4$  and  $e_5$ . Let us check all five cases:

- If no edge  $e_k$  is a bridge, then  $P - t$  is elementary.
- If only  $e_4$  is a bridge, then it splits  $P$  into two components. This means that  $P$  is formed by the merging of two elementary  $(\{2, 3\}, 5)$ -polycycles.
- If  $e_3$  or  $e_5$  is a bridge, then  $P - t$  is formed by the agglomeration of an elementary  $(\{2, 3\}, 5)$ -polycycle and a  $i$ -gon with  $i = 2$  or  $3$ .
- If  $e_4$  is a bridge and  $e_3$  or  $e_5$  is a bridge, then  $P - t$  is formed by the agglomeration of an elementary  $(\{2, 3\}, 5)$ -polycycle and two  $i$ -gons with  $i = 2$  or  $3$ .
- If all  $e_k$  are bridges, then  $P$  has only one interior vertex.

Given a hole of a  $(R, q)$ -polycycle, its *boundary sequence* is the sequence of degrees of all consecutive vertices of the boundary of this hole. It is a slight generalization of Chapter 5, where the considered polycycles have only one exterior face.

**Theorem 7.6.1** *The list of elementary  $(\{2, 3\}, 5)_{gen}$ -polycycles consists of:*

- (i) 57 sporadic  $(\{2, 3\}, 5)$ -polycycles given in Appendix 2,
- (ii) three following infinite  $(\{2, 3\}, 5)$ -polycycles:



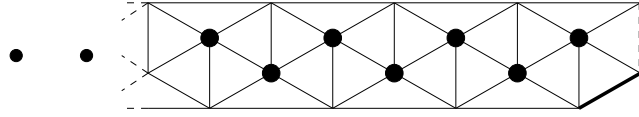
- (iii) Six infinite series of  $(\{2, 3\}, 5)$ -polycycles with one hole (they are obtained by concatenating endings of a pair of polycycles, given in (ii); see Figure 7.5 for the first 5 graphs),
- (iv) the infinite series of snub  $APrism_m$ , for  $2 \leq m \leq \infty$ , and its non-orientable quotients for  $m$  odd.

**Proof.** Let us take an elementary  $(\{2, 3\}, 5)$ -polycycle, which is finite. Then, by removing a 3-gon, which is adjacent to a boundary, one is led to the situation described above. Hence, the algorithm for enumerating finite elementary  $(\{2, 3\}, 5)$ -polycycles is the following:

1. Begin with isolated  $i$ -gons with  $i = 2$  or  $3$ .
2. For every vertex  $v$  of an elementary polycycle with  $n$  interior vertices, consider all possibilities of adding 2- and 3-gons incident to  $v$ , such that the obtained polycycle is elementary and  $v$  has become an interior vertex.
3. Reduce by isomorphism.

The above algorithm first finds some sporadic elementary  $(\{2, 3\}, 5)$ -polycycles and the first elements of the infinite series and then find only the elements of the infinite series. In order to prove that this is the complete list of all finite elementary  $(\{2, 3\}, 5)$ -polycycles, one needs to consider the case, in which only  $e_4$  is a bridge going from a hole to the same hole. So, one needs to consider all possibilities, where the addition of two elementary  $(\{2, 3\}, 5)$ -polycycles and one 3-gon makes a larger elementary  $(\{2, 3\}, 5)$ -polycycle. Given a sequence  $a_1, \dots, a_n$ , say that a sequence  $b_1, \dots, b_p$  with  $p < n$  is a *pattern* of that sequence if, for some  $n_0$ , one has  $a_{n_0+j-1} = b_j$  or  $a_{n_0+1-j} = b_j$  with the addition being modulo  $n$ . The  $(\{2, 3\}, 5)$ -polycycles, used in that construction, should have the pattern  $3, 3, x$  with  $x \leq 4$  in their boundary sequence. Only the polycycles, which belong to the six infinite series, satisfy this and it is easy to see, that the result of the operation is still one of the six infinite series. So, the list of finite elementary  $(\{2, 3\}, 5)$ -polycycles is given in the theorem.

Consider now an elementary infinite  $(\{2, 3\}, 5)$ -polycycle  $P$ . Eliminate all 2-gonal faces of  $P$  and obtain another  $(3, 5)$ -polycycle  $P'$ , which is not necessarily elementary. We do a decomposition of  $P'$  along its elementary components, which are enumerated in Section 7.3. If snub  $APrism_\infty$  is one of the components, then we are finished and  $P = P'$  is snub  $APrism_\infty$ . If  $\alpha$  is one of the components, then one has two edges, along which one can extend the polycycle; they are depicted below:



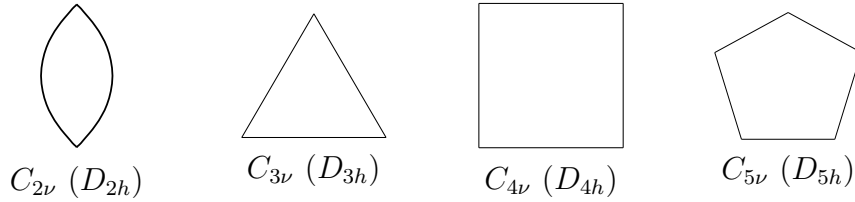
Clearly, if one extends the polycycle along only one of those edges, then the result is not an elementary polycycle. The consideration of all possibilities yields  $\beta$  and  $\gamma$ . Suppose now that  $P'$  has no infinite components. Then  $P$  has at least one infinite path  $f_0, \dots, f_i, \dots$ , such that  $f_i$  is adjacent to  $f_{i+1}$ , but  $f_{i-1}$  is not adjacent to  $f_{i+1}$ . The considerations, analogous to the 3-valent case, yield the result for  $(\{2, 3\}, 5)$ -polycycles.

If  $P$  is an elementary  $(\{2, 3\}, 5)_{gen}$ -polycycle, which is not a  $(\{2, 3\}, 5)$ -polycycle then its universal cover  $\tilde{P}$  is an elementary  $(\{2, 3\}, 5)$ -polycycle which has a fixed-point-free automorphism group included in  $Aut(\tilde{P})$ . Clearly, only snub  $APrism_\infty$  is such and it yields the infinite series of snub  $APrism_m$  and its non-orientable quotients.  $\square$

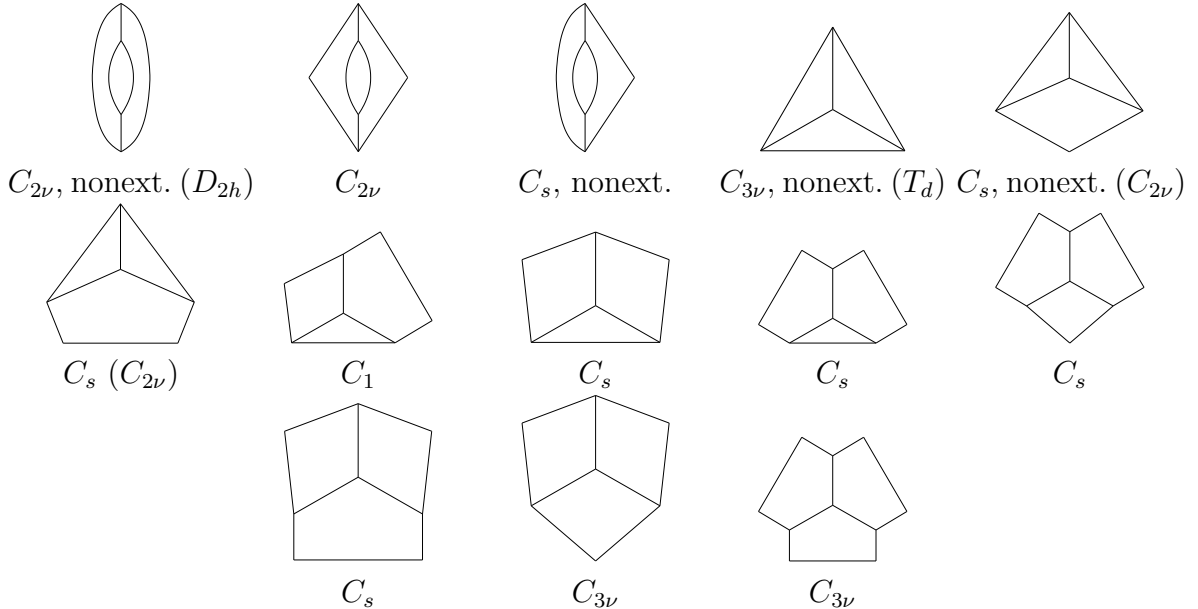
## 7.7 Appendix 1: 204 Sporadic elementary $(\{2, 3, 4, 5\}, 3)$ -polycycles

Below (11 cases), when several elementary sporadic  $(\{2, 3, 4, 5\}, 3)$ -polycycles correspond to the same plane graph, we always add the sign  $\mathbf{x}$  with  $1 \leq x \leq 11$ .

List of 4 sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles with 1 proper face:

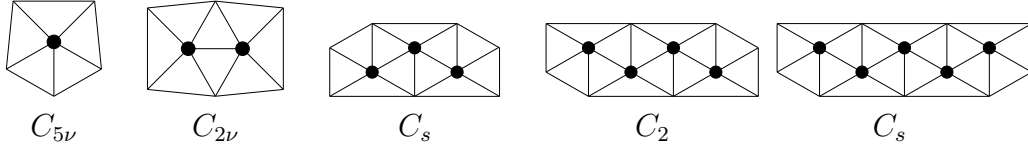


List of 13 sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles with 3 proper faces:

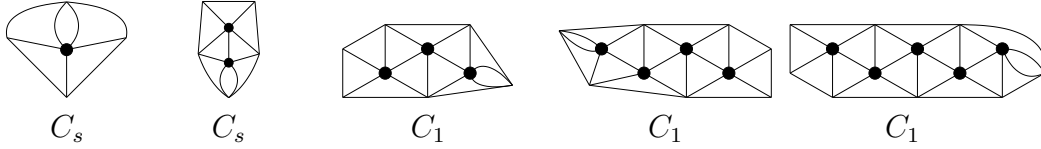


List of 26 sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles with 4 proper faces:

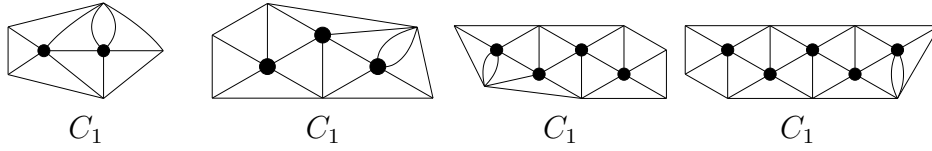
Infinite series  $\alpha\alpha$  of elementary  $(\{2,3\},5)$ -polycycles ( $e_1$ - $e_6$ ):



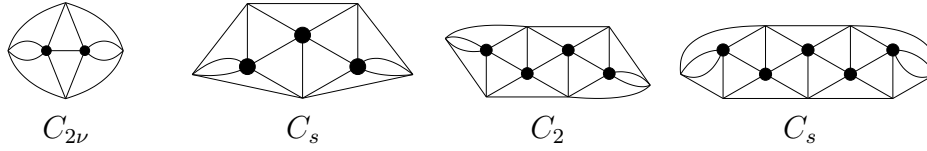
Infinite series  $\alpha\beta$  of elementary  $(\{2,3\},5)$ -polycycles:



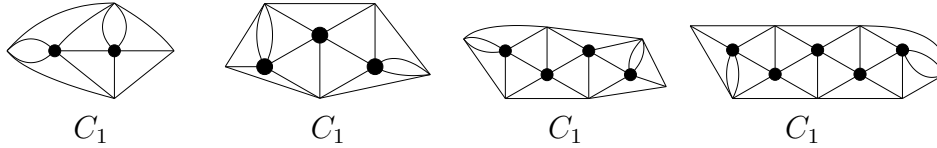
Infinite series  $\alpha\gamma$  of elementary  $(\{2,3\},5)$ -polycycles:



Infinite series  $\beta\beta$  of elementary  $(\{2,3\},5)$ -polycycles:



Infinite series  $\beta\gamma$  of elementary  $(\{2,3\},5)$ -polycycles:



Infinite series  $\gamma\gamma$  of elementary  $(\{2,3\},5)$ -polycycles:

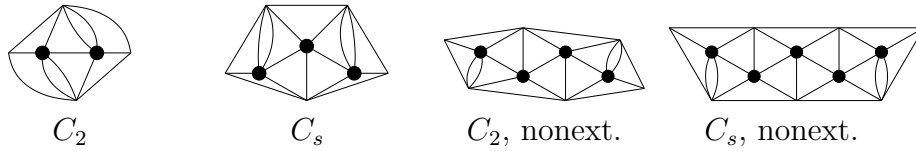
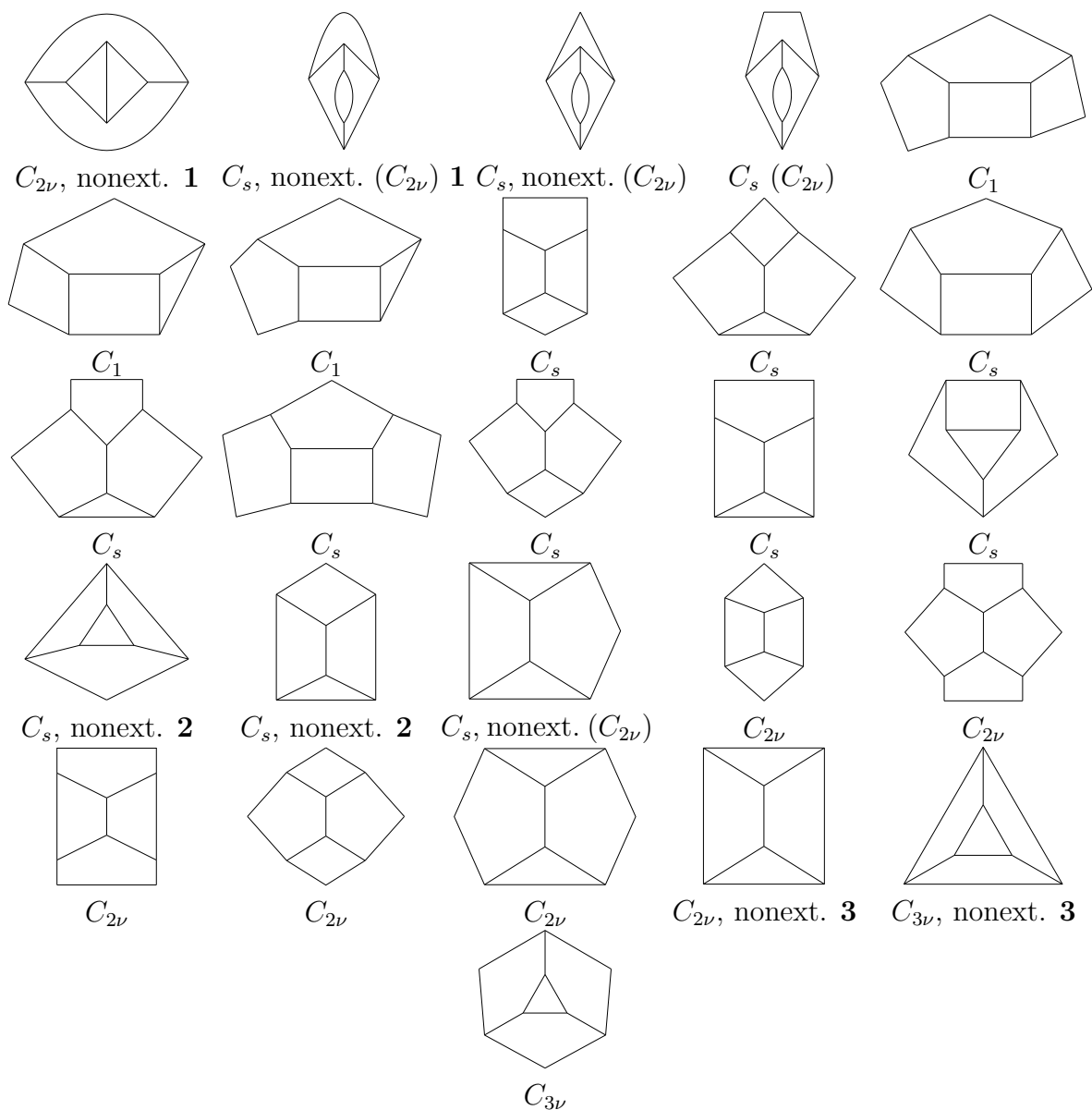
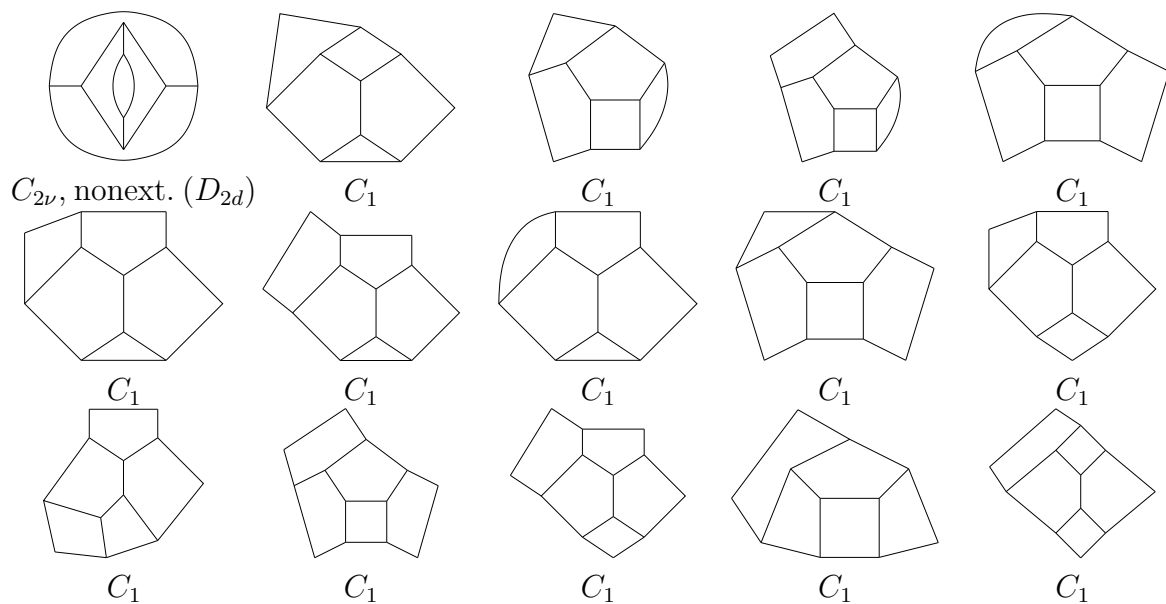
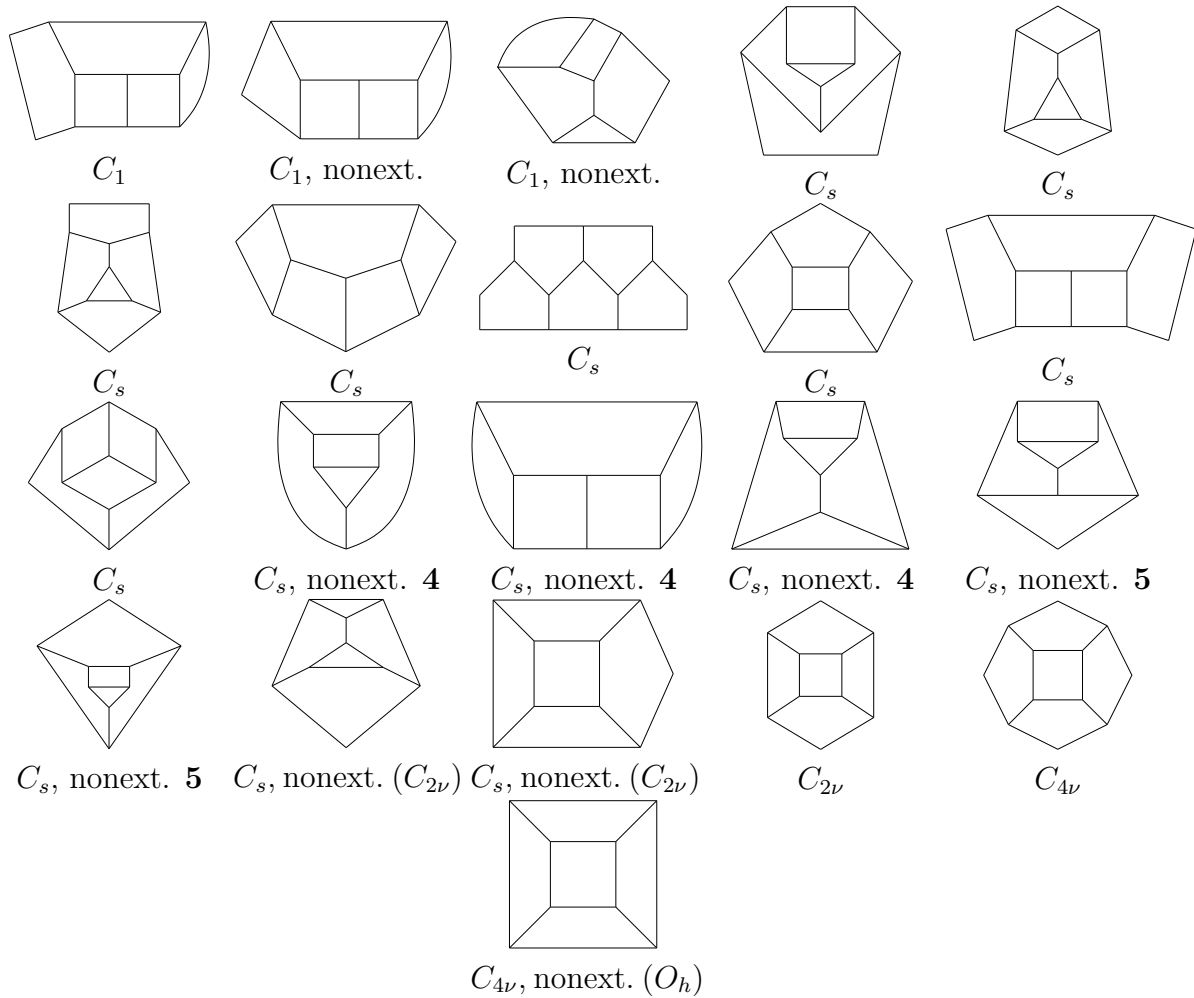


Figure 7.5: The first 5 members of the six infinite series of  $(\{2,3\},5)$ -polycycles

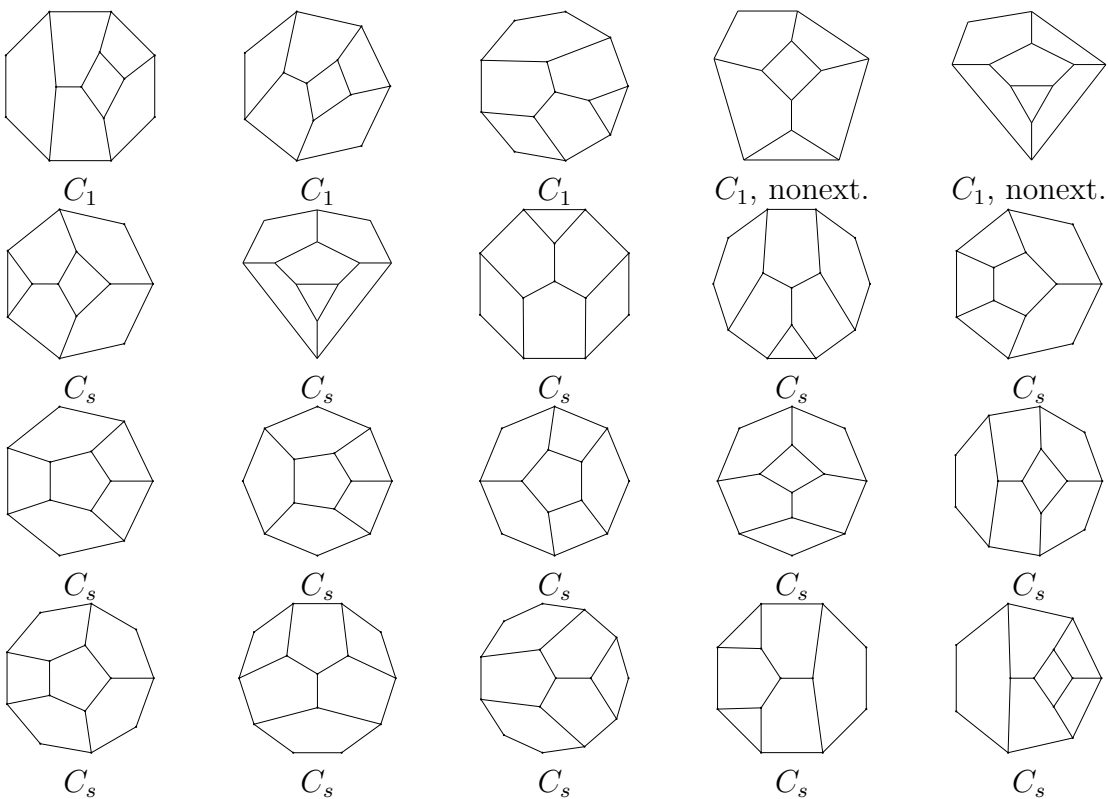


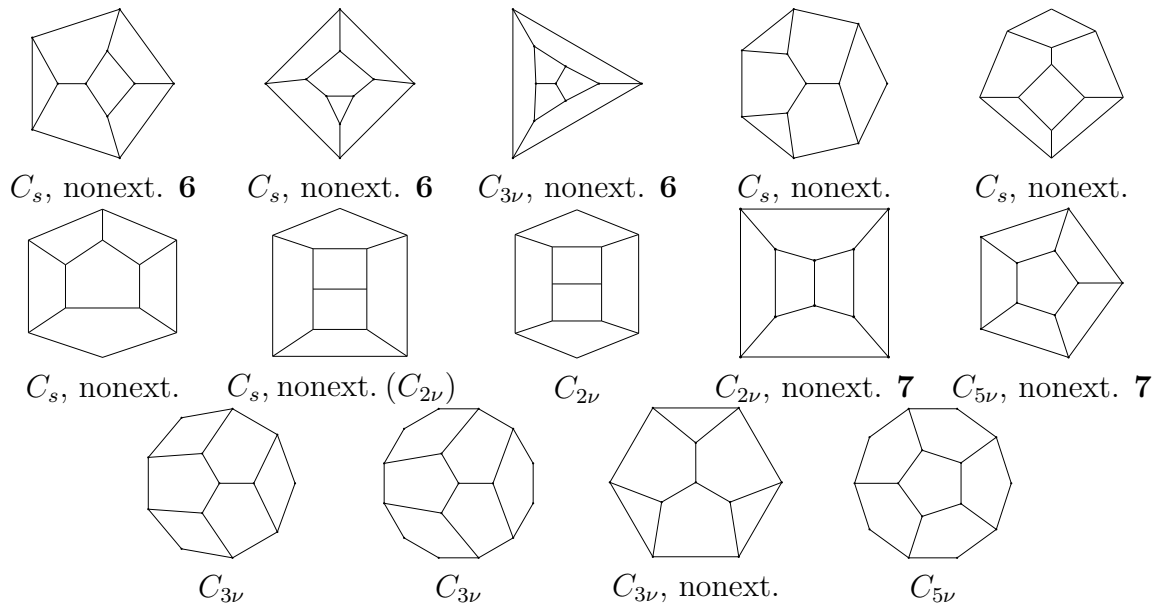
List of 36 sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles with 5 proper faces:



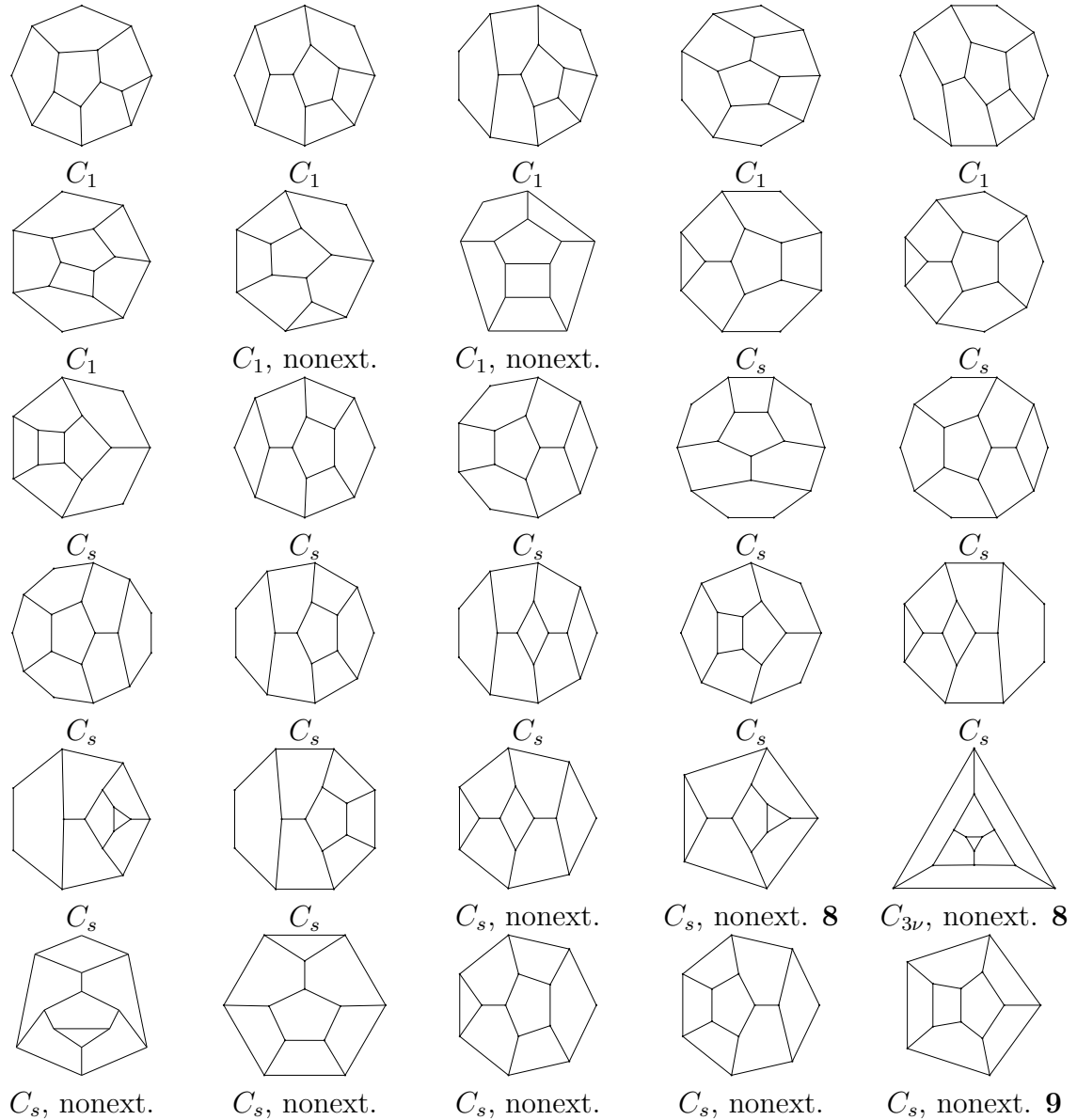


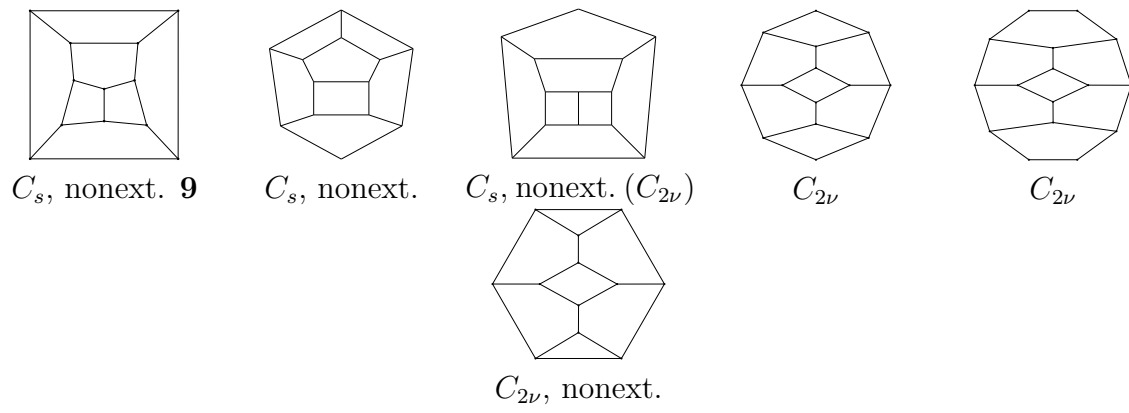
List of 34 sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles with 6 proper faces:



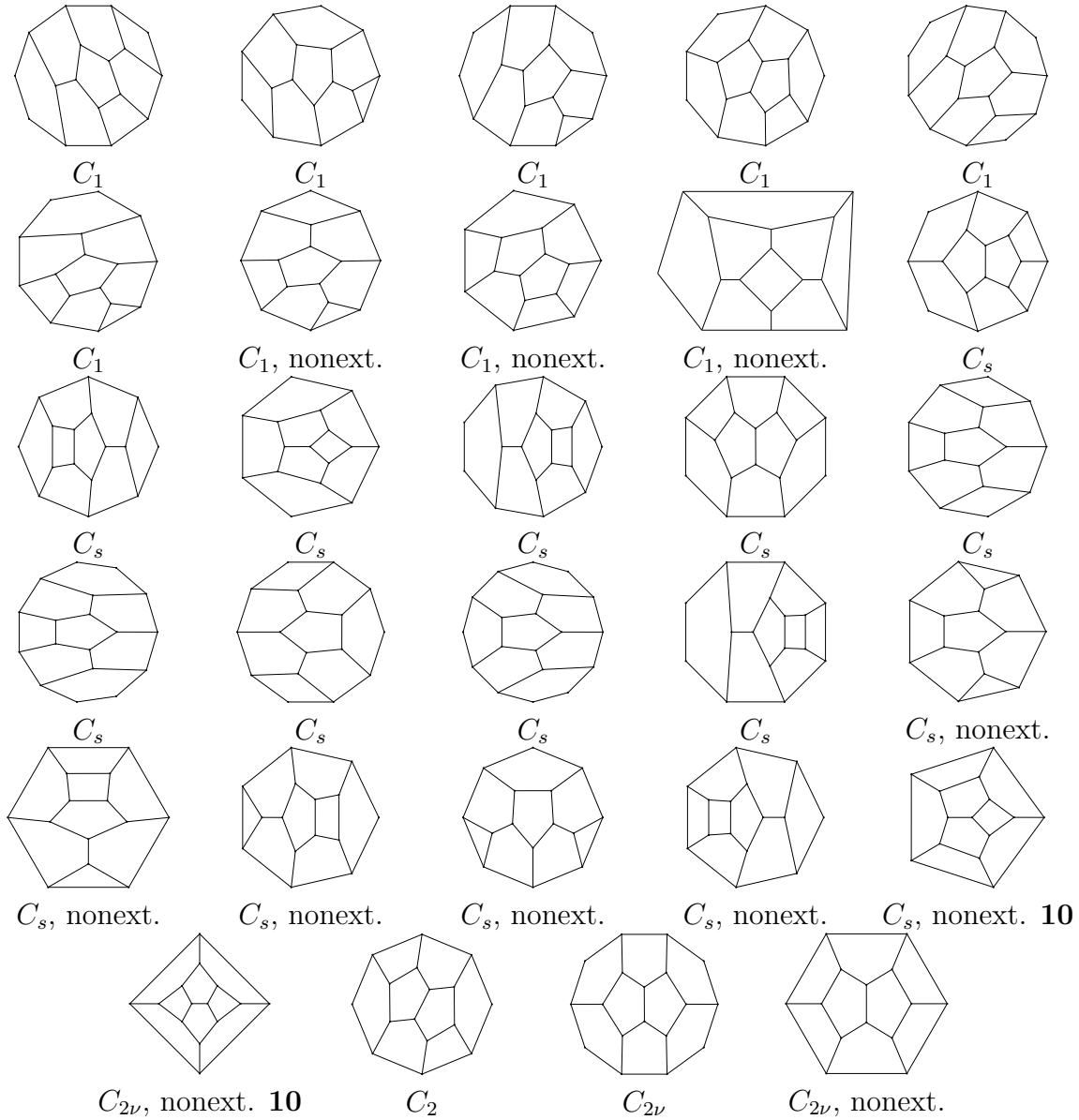


List of 36 sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles with 7 proper faces:

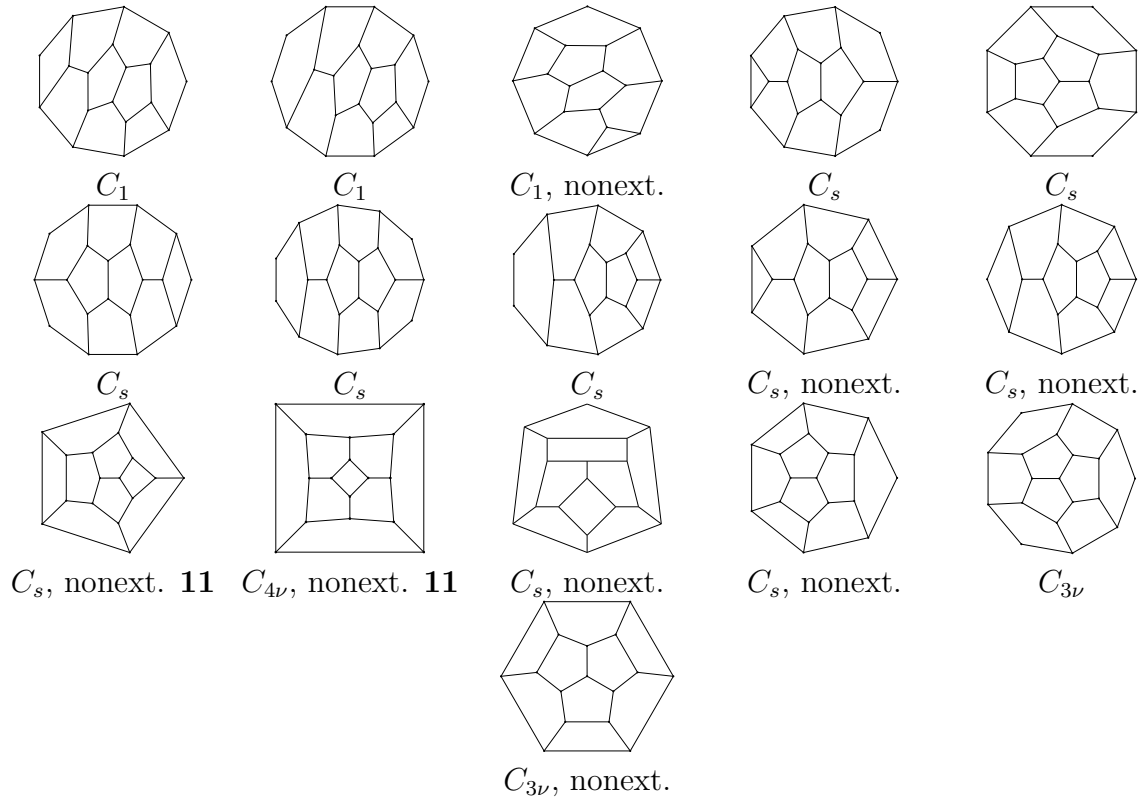




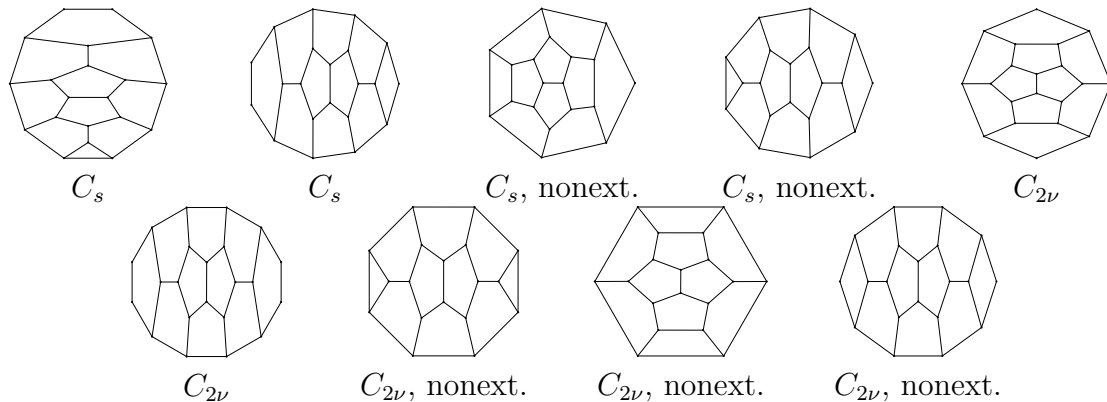
List of 29 sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles with 8 proper faces:



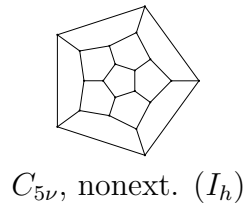
List of 16 sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles with 9 proper faces:



List of 9 sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycles with 10 proper faces:



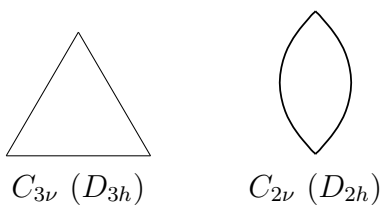
Unique sporadic elementary  $(\{2, 3, 4, 5\}, 3)$ -polycycle with at least 11 proper faces:



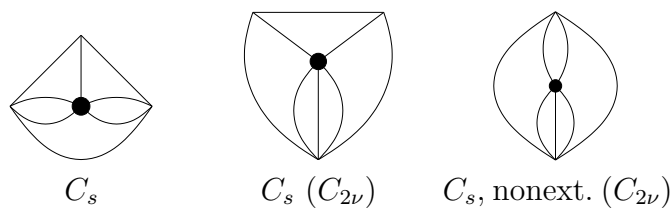
## 7.8 Appendix 2: 57 sporadic elementary $(\{2, 3\}, 5)$ -polycycles

Below (three cases) when several elementary sporadic  $(\{2, 3\}, 5)$ -polycycles correspond to the same plane graph, we always add the sign **A**, **B** or **C**.

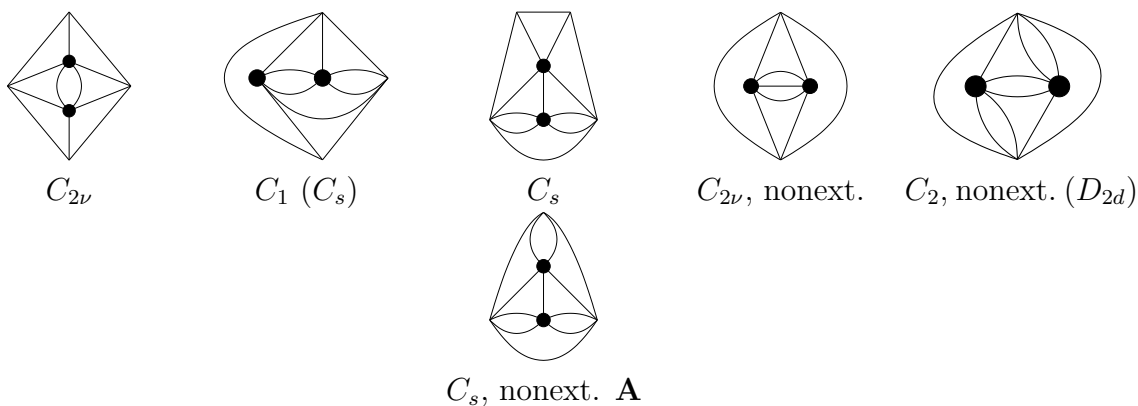
List of 2 sporadic elementary  $(\{2, 3\}, 5)$ -polycycles without interior vertices:



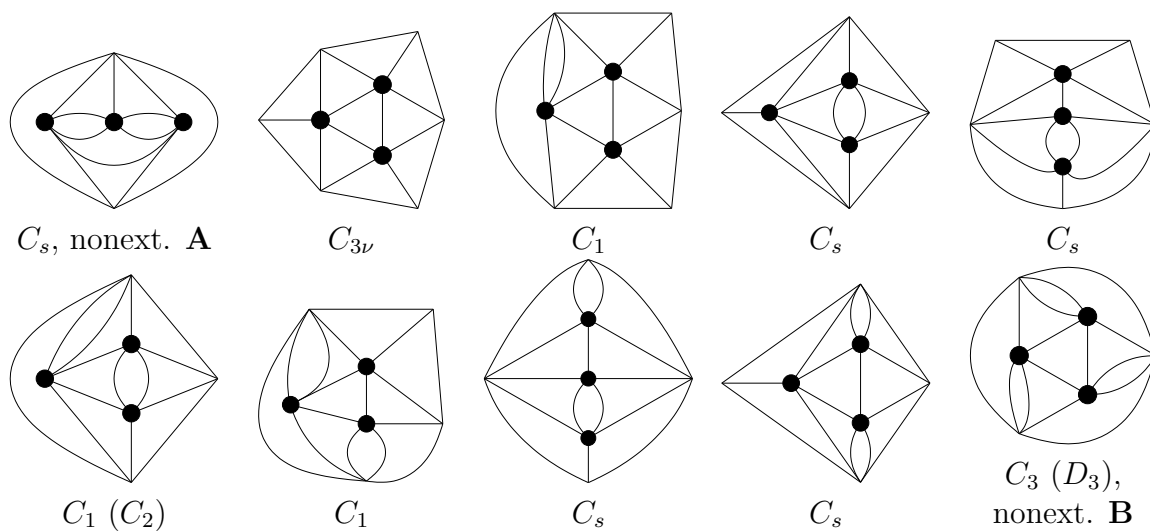
List of 3 sporadic elementary  $(\{2, 3\}, 5)$ -polycycles with 1 interior vertex:



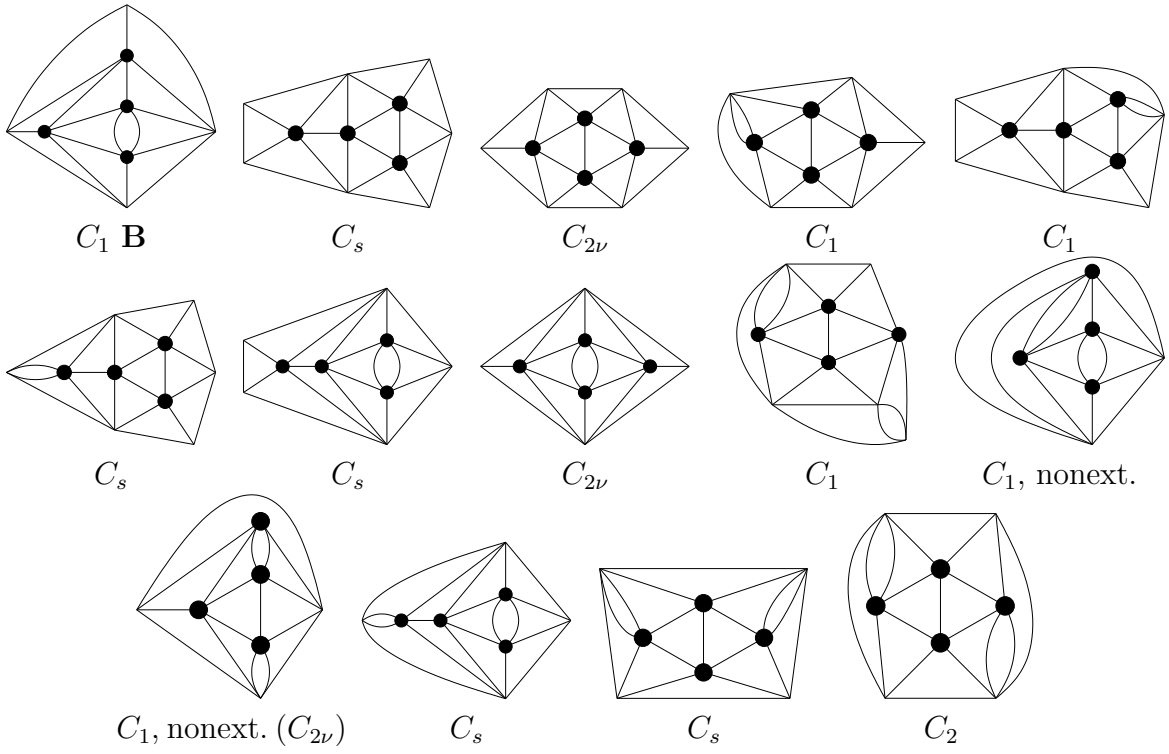
List of 6 sporadic elementary  $(\{2, 3\}, 5)$ -polycycles with 2 interior vertices:



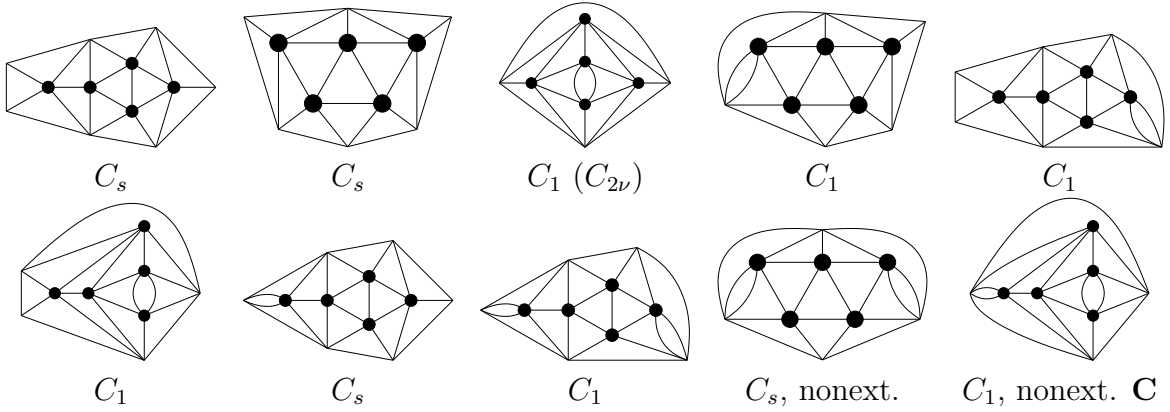
List of 10 sporadic elementary  $(\{2, 3\}, 5)$ -polycycles with 3 interior vertices:



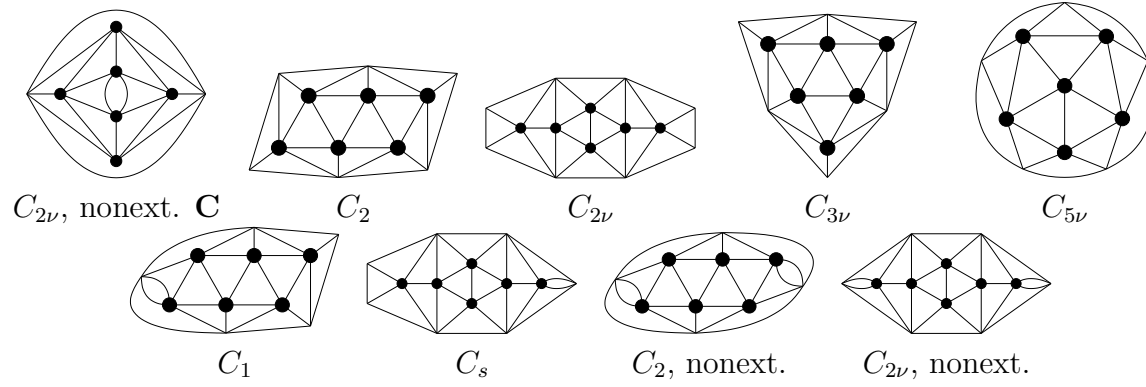
List of 14 sporadic elementary  $(\{2, 3\}, 5)$ -polycycles with 4 interior vertices:



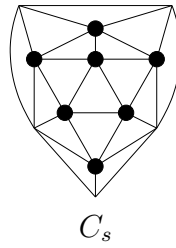
List of 10 sporadic elementary  $(\{2, 3\}, 5)$ -polycycles with 5 interior vertices:



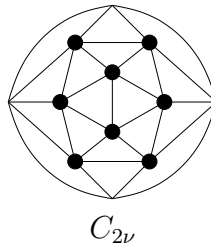
List of 9 sporadic elementary  $(\{2, 3\}, 5)$ -polycycles with 6 interior vertices:



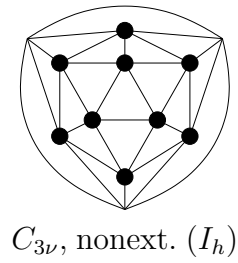
Unique sporadic elementary  $(\{2, 3\}, 5)$ -polycycle with 7 interior vertices:



Unique sporadic elementary  $(\{2, 3\}, 5)$ -polycycle with 8 interior vertices:



Unique sporadic elementary  $(\{2, 3\}, 5)$ -polycycle with at least 9 interior vertices:



# Chapter 8

## Applications of elementary decompositions to $(r, q)$ -polycycles

We present here applications of elementary polycycle decomposition (in particular, of lists in Figures 7.2 and 7.3) to three problems:

1. The determination of  $(r, q)$ -polycycles having maximal number of interior vertices for fixed number of interior faces. Complete solution for the elliptic case is presented.
2. The determination of all *non-extensible*  $(r, q)$ -polycycles, i.e., ones which cannot be extended by adding an  $r$ -gon. In particular, besides 5 Platonic cases and 2 exceptional elliptic polycycles, they are infinite.
3. The determination of 2-embeddable  $(r, q)$ -polycycles, i.e., ones whose skeleton can be embedded into a hypercube with scale 2. All parabolic and hyperbolic  $(r, q)$ -polycycles are 2-embeddable and a characterization (by extended subgraphs of) such elliptic  $(r, q)$ -polycycles is presented.

None of those applications are considered for other classes of polycycles, like  $(R, q)$ -polycycles and  $(r, q)_{gen}$ -polycycles. A fourth main application, to face-regular maps, will be considered in Chapters 12, 13, 14, 18.

Given an  $(r, q)_{gen}$ -polycycle  $P$ , its *major skeleton*  $Maj(P)$  is the plane graph formed by its elementary components with two components being adjacent if they share an open edge. A *tree* is a connected graph with no cycles.

**Theorem 8.0.1** *An  $(r, q)_{gen}$ -polycycle  $P$  is simply connected, i.e., is an  $(r, q)$ -polycycle, if and only if it holds:*

- (i) *its elementary components are simply connected and*
- (ii) *its major skeleton  $Maj(P)$  is a tree.*

**Proof.** Assume (i) and (ii) hold, and take a closed cycle  $c$  in  $P$ . The set of elementary polycycles, passed by  $c$ , is a finite connected subgraph  $Maj_c(P)$  of  $Maj(P)$ , so, a tree also. If  $c$  pass through only one elementary component, then, by (i), we are done. Suppose that  $c$  pass through more than one elementary component, then one vertex of  $Maj_c(P)$  is of degree 1. Denote by  $e$  the open edge connecting the elementary component to the rest of  $Maj_c(P)$ . By (i), one can continuously transform  $c$  into a path  $c'$  that pass only

thought  $e$ , i.e., eliminate one vertex of  $Maj_c(P)$ . Iterating, we are led to  $Maj_c(P)$  being a single vertex and one concludes again by (i).

Condition (i) is, clearly, necessary. If (ii) is not satisfied, then  $Maj(P)$  contains a cycle. This cycle corresponds to a cycle in  $P$ , which, clearly, is not homotopic to 0.  $\square$

## 8.1 Extremal polycycles

Denote by  $p_r(P)$ ,  $v_{int}(P)$  (or, simply,  $p_r$ ,  $v_{int}$ ) the number of interior faces and interior vertices of given finite  $(r, q)$ -polycycle  $P$ . Denote by  $dens(P)$  and call *density* of a finite  $(r, q)$ -polycycle  $P$  the quotient  $dens(P) = \frac{v_{int}(P)}{p_r(P)}$ . Denote by  $N_{r,q}(x)$  the maximum of  $v_{int}(P)$  over all  $(r, q)$ -polycycles  $P$  with  $p_r(P) = x$ ; call *extremal* any  $(r, q)$ -polycycle  $P$  with  $v_{int}(P) = N_{r,q}(x)$ . So, extremal polycycles represent the opposite case to outerplanar ones, in the class of all  $(r, q)$ -polycycles with the same  $p_r$ .

**Remark 8.1.1** *Amongst all  $(r, q)$ -polycycles with the same  $p_r$ , the following are equivalent:*

1.  $v_{int}$  is maximal,
2.  $e_{int}$  (the number of non-boundary edges) is maximal,
3. the perimeter  $Per$  (the number of boundary edges) is minimal,
4. the number  $v$  of vertices is minimal,
5. the number  $e$  of edges is minimal.

This follows easily from Euler formula  $(v_{int} + Per) - (e_{int} + Per) + (p_r + 1) = 2$  and equality  $rp_r = 2e_{int} + Per$ .

For  $(5, 3)$ -polycycles with  $x \leq 11$ ,  $N_{5,3}(x)$  was found in [CCBBZGT93]; all such extremal  $(5, 3)$ -polycycles turn out to be proper and unique. Moreover, the  $(5, 3)$ -polycycles, which are reciprocal (see Section 4.1) to any such extremal one, turn out to be also extremal. [CCBBZGT93] asked about  $N_{5,3}(x)$  for  $x \geq 12$ ; this section answers this question for any  $x$  and for all elliptic  $(p, q)$ .

In spite of the negative result of Theorem 7.2.1, one can easily obtain the following general density estimate.

**Theorem 8.1.2** *(i) For any finite  $(r, q)$ -polycycle  $P$ , it holds:*

$$dens(P) < \frac{r}{q}.$$

*(ii) For parabolic  $(r, q)$ , there exists a sequence of  $(r, q)$ -polycycles  $P_v$  with:*

$$\lim_{v \rightarrow \infty} dens(P_v) = \frac{r}{q}.$$

**Proof.** (i) Take an arbitrary  $(r, q)$ -polycycle  $P$ . We tile each  $r$ -gon into 4-gons by connecting its center with the midpoints of the sides. Then the number of 4-gons in each  $r$ -gon is equal to  $r$  and the number of 4-gons, incident to any internal vertex, is equal to  $q$ . Then the number of 4-gons, incident only to internal vertices of the polycycle  $P$ , is equal to  $v_{int}q$ , while the total number of 4-gons is equal to  $rp_r$ . Hence,  $v_{int}q < rp_r$ .

(ii) On the Euclidean plane  $\{r, q\}$ , take a disk  $C(0, R)$  with center 0 and radius  $R$ . Define the  $(r, q)$ -polycycle  $P_R$  to be formed by all  $r$ -gons contained in  $C(0, R)$ . It is easy to see that  $\lim_{R \rightarrow \infty} dens(P_R) = \frac{r}{q}$ .  $\square$

All  $(3, 3)$ -,  $(4, 3)$ -, and  $(3, 4)$ -polycycles were obtained in [Har90] (proper) and [DeSt98] (improper ones). In the case of  $(r, q) = (3, 3)$ , the pairs  $(p_r, v_{int})$  are  $(1, 0)$ ,  $(2, 0)$ , and  $(3, 1)$ ; in the case of  $(r, q) = (4, 3)$ , the pairs  $(p_r, v_{int})$  are  $(m, 0)$  for any  $m \geq 1$ ,  $(|\mathbb{N}|, 0)$  and<sup>1</sup>  $(|\mathbb{Z}|, 0)$ ,  $(3, 1)$ ,  $(4, 2)$ , and  $(5, 4)$ ; in the case of  $(r, q) = (3, 4)$ , the pairs  $(p_r, v_{int})$  are  $(m, 0)$  for any  $m \geq 1$ ,  $(|\mathbb{N}|, 0)$  and  $(|\mathbb{Z}|, 0)$ ,  $(4, 1)$ ,  $(5, 1)$ ,  $(6, 1)$ ,  $(6, 2)$ , and  $(7, 3)$ . Amongst these pairs, those with  $v_{int} \geq 1$ , except for the pair  $(p_r, v_{int}) = (6, 1)$ , are realized only by proper polycycles; all improper polycycles, except for the case  $(p_r, v_{int}) = (6, 1)$ , have  $v_{int} = 0$ ; i.e., they are outerplanar.

**Theorem 8.1.3** *If a  $(r, q)$ -polycycle  $P$  is decomposed into elementary  $(r, q)$ -polycycles  $(EP_i)_{i \in I}$  appearing  $x_i$  times, then one has:*

$$\begin{cases} v_{int}(P) &= \sum_{i \in I} x_i v_{int}(EP_i) \\ p_r(P) &= \sum_{i \in I} x_i p_r(EP_i). \end{cases}$$

If one solves the linear programming problem:

$$\begin{aligned} &\text{maximize} && \sum_{i \in I} x_i v_{int}(EP_i) \\ &\text{with} && x = \sum_{i \in I} x_i p_r(EP_i) \\ &&& \text{and } x_i \in \mathbb{N} \end{aligned}$$

and if  $(x_i)_{i \in I}$ , realizing the maximum, can be realized as  $(r, q)$ -polycycle, then  $N_{r,q}(x)$  is equal to the value of the objective function.

If this is not the case, then we have more possibilities to consider.

### 8.1.1 Extremal $(5, 3)$ -polycycles

**Theorem 8.1.4** (i) *If  $x \leq 12$ , then  $N_{5,3}(x)$  is as given in Figure 8.1 with all the extremal  $(5, 3)$ -polycycles realizing the extremum.*

(ii) *For any  $x \geq 12$ , one has:*

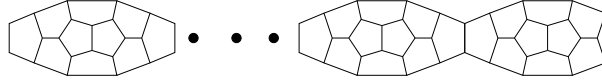
$N_{5,3}(x) = x$  if  $x \equiv 0, 8, 9 \pmod{10}$  with the maximum realized by the following unique extremal  $(5, 3)$ -polycycle:

- If  $x \equiv 0 \pmod{10}$ , it is  $\frac{x}{10}C_1$ :



<sup>1</sup>Here we distinguish two cases that are formally denoted by  $(|\mathbb{N}|, 0)$  and  $(|\mathbb{Z}|, 0)$  depending on whether a polycycle (considered as a chain) is infinite only in one direction or in two opposite directions.

- If  $x \equiv 9 \pmod{10}$ , it is  $\frac{x-9}{10}C_1 + B_2$ :

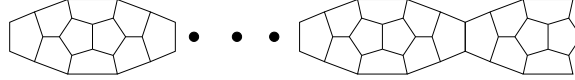


- If  $x \equiv 8 \pmod{10}$ , it is  $B_2 + \frac{x-18}{10}C_1 + B_2$ :



$N_{5,3}(x) = x - 1$  if  $x \equiv 6, 7 \pmod{10}$  with the maximum realized by the following (non-unique) extremal  $(5, 3)$ -polycycle:

- If  $x \equiv 7 \pmod{10}$ , it is  $\frac{x-7}{10}C_1 + B_3$ :



- If  $x \equiv 6 \pmod{10}$ , it is  $B_2 + \frac{x-16}{10}C_1 + B_3$ :



$N_{5,3}(x) = x - 2$  if  $x \equiv 1, 2, 3, 4, 5 \pmod{10}$  and the extremum is realized by (non-unique)  $E_{x+2}$ .

(iii) All possible densities of finite  $(5, 3)$ -polycycles, except for three cases  $p_5 = 9, 10, 11$  are all rational numbers of the segment  $[0, 1]$ . All possible densities of polycycles, any of whose faces contain an internal vertex, are all rational numbers of the segment  $[\frac{1}{3}, 1]$ .

**Proof.** The proof of (i) and (ii) uses decomposition of  $(5, 3)$ -polycycles into elementary ones and the classification of elementary  $(5, 3)$ -polycycles. For example, for  $p_5 \equiv 0 \pmod{10}$ , an extremal polycycle is obtained by gluing only the copies of the polycycle  $C_1$ , while, for  $p_5 \equiv 9 \pmod{10}$  or  $p_5 \equiv 8 \pmod{10}$ , one should glue together the copies of the polycycle  $C_1$  and one or two copies of the polycycle  $B_2$  (always at a deadlock). An elementary polycycle  $E_{x-2}$  is extremal for  $n(x) = x - 2 \geq 10$ ; however, even for  $x = 12$ , there are three other extremal  $(5, 3)$ -polycycles.

The  $(5, 3)$ -polycycles  $E_1$ ,  $C_1$  have densities  $\frac{1}{3}$ , 1, respectively. Furthermore, if  $P$  is a  $(5, 3)$ -polycycle of the form  $mE_1 + nC_1$ , then its density is:

$$\text{dens}(P) = \frac{m + 10n}{3m + 10n}.$$

It is easy to see that one can find  $n, m \in \mathbb{N}$  realizing all rational densities in  $[\frac{1}{3}, 1]$ . If every 5-gon is incident to an interior vertex, then  $E_1$  does not occur as elementary component of  $P$ . If  $p_5 \geq 12$ , then  $A_i$  cannot occur as elementary component. All remaining elementary components have densities between  $\frac{1}{3}$  and 1, thereby proving that for  $p_5 \notin \{9, 10, 11\}$  the densities belong to  $[\frac{1}{3}, 1]$ . If one allows for the polycycle  $D$  to occur, then all rational densities in  $[0, 1]$  can be realized.  $\square$

As  $x$  grows the number of extremal polycycles in the non-unique cases grows. For example, for  $x = 13, 14$ , and 15, the polycycles  $C_1 + E_1$ ,  $C_1 + E_2$ , and  $C_1 + E_3$  are also extremal. It would be interesting to extend the notion of densities to infinite  $(r, q)$ -polycycles, but it is sometimes impossible to define densities for infinite settings (see [FeKuKu98, FeKu93], for hyperbolic space).

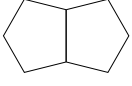
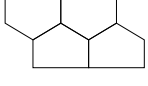
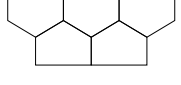
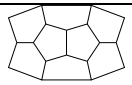
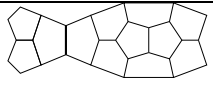
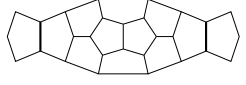
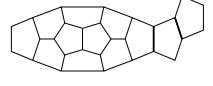
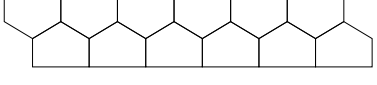
| $x$ | $N_{5,3}(x)$ | extremal polycycles                                                                                                                                                                                                                                                                                                                                       | components                                                |
|-----|--------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------|
| 1   | 0            |                                                                                                                                                                                                                                                                          | $D$                                                       |
| 2   | 0            |                                                                                                                                                                                                                                                                          | $2D$                                                      |
| 3   | 1            |                                                                                                                                                                                                                                                                          | $E_1$                                                     |
| 4   | 2            |                                                                                                                                                                                                                                                                          | $E_2$                                                     |
| 5   | 3            |                                                                                                                                                                                                                                                                          | $E_3$                                                     |
| 6   | 5            |                                                                                                                                                                                                                                                                          | $A_5$                                                     |
| 7   | 6            |                                                                                                                                                                                                                                                                          | $B_3$                                                     |
| 8   | 8            |                                                                                                                                                                                                                                                                          | $A_4$                                                     |
| 9   | 10           |                                                                                                                                                                                                                                                                         | $A_3$                                                     |
| 10  | 12           |                                                                                                                                                                                                                                                                        | $A_2$                                                     |
| 11  | 15           |                                                                                                                                                                                                                                                                        | $A_1$                                                     |
| 12  | 10           | <br><br><br> | $E_1 + B_2$<br>$D + C_1 + D$<br>$C_1 + D + D$<br>$E_{10}$ |

Figure 8.1: Extremal  $(5, 3)$ -polycycles with at most 12 faces

### 8.1.2 Extremal (3, 5)-polycycles

**Theorem 8.1.5** (i) If  $x \leq 19$ , then  $N_{3,5}(x)$  is as given in Figure 8.2 with all the extremal (5, 3)-polycycles realizing the extremum.

(ii) For any  $x \geq 20$ , one has:

| $x \equiv a \pmod{18}$ | $N_{3,5}(x)$    | extremal polycycles                                                   | unicity |
|------------------------|-----------------|-----------------------------------------------------------------------|---------|
| $a = 0$                | $\frac{x}{3}$   | $\frac{x}{18}b_2$                                                     | no      |
| $a = 1$                | $\frac{x-1}{3}$ | $d + \frac{x-1}{18}b_2$                                               | no      |
| $a = 10$               | $\frac{x-1}{3}$ | $b_3 + \frac{x-28}{18}b_2 + b_4$<br>$\frac{x-10}{18}(c_1 + 2d) + c_4$ | no      |
| $a = 12$               | $\frac{x}{3}$   | $b_3 + \frac{x-30}{18}b_2 + b_3$<br>$\frac{x-12}{18}(c_1 + 2d) + c_3$ | no      |
| $a = 13$               | $\frac{x-1}{3}$ | $b_4 + \frac{x-13}{18}b_2$                                            | yes     |
| $a = 14$               | $\frac{x+1}{3}$ | $\frac{x-14}{18}(c_1 + 2d) + c_2$                                     | no      |
| $a = 15$               | $\frac{x}{3}$   | $b_3 + \frac{x-15}{18}b_2$                                            | yes     |
| $a = 16$               | $\frac{x+2}{3}$ | $\frac{x-16}{18}(c_1 + 2d) + c_1$                                     | yes     |
| $a = 17$               | $\frac{x+1}{3}$ | $\frac{x-17}{18}(c_1 + 2d) + c_1 + d$                                 | yes     |

and, if  $x$  is not listed above, then the following applies:

| $x \equiv a \pmod{3}$ | $N_{3,5}(x)$    | extremal polycycles   | unicity |
|-----------------------|-----------------|-----------------------|---------|
| $a = 2$               | $\frac{x-2}{3}$ | $e_{N_{3,5}(x)}$      | no      |
| $a = 0$               | $\frac{x-3}{3}$ | $d + e_{N_{3,5}(x)}$  | no      |
| $a = 1$               | $\frac{x-4}{3}$ | $2d + e_{N_{3,5}(x)}$ | no      |

(iii) all possible densities of finite (3, 5)-polycycles, except for  $x \in \{14, \dots, 19\}$  are all rational numbers of the segment  $[0, \frac{1}{3}]$ .

**Proof.** To prove Theorem 8.1.5, we apply the same strategy as for Theorem 8.1.4 except that now the number of cases to consider is larger (see Figure 7.3 of elementary (3, 5)-polycycles and their kernels).

For  $x \leq 19$ , the enumeration is done by hand since it contains some sporadic cases. For other values of  $x$ , one first remarks that the  $a_i$  and  $b_1$  cannot be elementary components of extremal polycycles. Afterward, one does exhaustive enumeration of all possibilities.  $\square$

### 8.1.3 Parabolic and hyperbolic extremal $(r, q)$ -polycycles

The results presented here are very partial, but we do not expect difficulty in obtaining general results.

For parabolic or hyperbolic parameters  $(r, q)$ , the *spiral*  $Sp_{r,q}(n)$  is defined as the proper  $(r, q)$ -polycycle with  $n$   $r$ -gons obtained by taking an  $r$ -gon and adding  $r$ -gons in sequence always rotating in the same direction. A formal definition is difficult to write (see [HaHa76, Gre01]); so, we show some examples below:

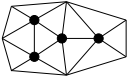
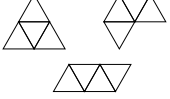
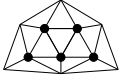
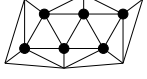
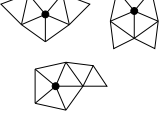
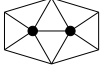
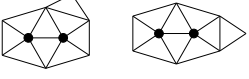
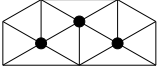
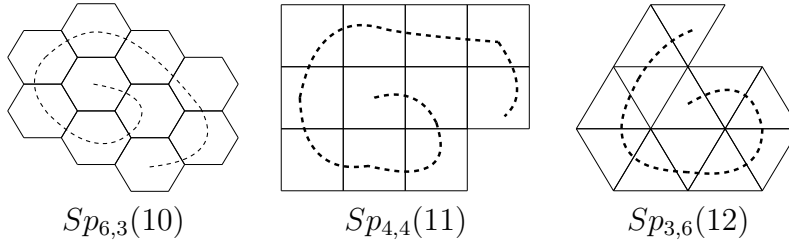
| $x$ | $N_{3,5}(x)$ | extremal                                                                            | comp.         | $x$ | $N_{3,5}(x)$ | extremal                                                                              | comp.     |
|-----|--------------|-------------------------------------------------------------------------------------|---------------|-----|--------------|---------------------------------------------------------------------------------------|-----------|
| 1   | 0            |    | $d$           | 12  | 4            |    | $c_3$     |
| 2   | 0            |    | $2d$          | 13  | 4            |    | $b_4$     |
| 3   | 0            |    | $3d$          |     |              |    | $b_4$     |
| 4   | 0            |    | $4d$          | 14  | 5            |    | $c_2$     |
| 5   | 1            |    | $e_1$         | 15  | 6            |    | $a_5$     |
| 6   | 1            |    | $e_1 + d$     | 16  | 6            |    | $c_1$     |
| 7   | 1            |   | $d + e_1 + d$ |     |              |   | $a_4$     |
| 8   | 2            |  | $e_2$         |     |              |  | $a_5 + d$ |
| 9   | 2            |  | $e_2 + d$     | 17  | 7            |  | $a_3$     |
| 10  | 3            |  | $c_4$         | 18  | 8            |  | $a_2$     |
| 11  | 3            |  | $e_3$         | 19  | 9            |  | $a_1$     |
|     |              |  | $c_4 + d$     |     |              |                                                                                       |           |

Figure 8.2: Extremal  $(3, 5)$ -polycycles with less than 20 faces



It is proved in [HaHa76] that, for parabolic  $(r, q)$ , the  $Sp_{r,q}(n)$  (called there *extremal animal*) is an  $(r, q)$ -polycycle with shortest perimeter amongst all proper  $(r, q)$ -polycycles. It is proved in [BBG03, Gre01] that, moreover,  $Sp_{6,3}(n)$  has shortest perimeter amongst all  $(6, 3)$ -polycycles. Remind, see previous section, that minimizing perimeter, when number of  $r$ -gons is fixed, is equivalent to maximizing the number of interior vertices.

It is conjectured that, for any parabolic or hyperbolic  $(r, q)$  and any  $n \geq 1$ ,  $Sp_{r,q}(n)$  is an extremal  $(r, q)$ -polycycle. A weaker conjecture is that all extremal polycycles are proper in non-elliptic case. Moreover, for hyperbolic  $(r, q)$ , it is likely that one has  $\frac{N_{r,q}(x)}{x} < C_{r,q}$  for some constant  $C_{r,q} < \frac{r}{q}$  (see Theorem 8.1.2 for the parabolic case). The reason would be that in hyperbolic space, the boundary is not negligible compared to the faces, which do not contain boundary edges; this point is well illustrated in [Mor97]. Also, the phenomenon, occurring in cases  $(r, q) = (5, 3)$  or  $(3, 5)$ , of having small  $(r, q)$ -polycycle with higher density  $\frac{N_{r,q}(x)}{x}$  than any other  $(r, q)$ -polycycle (for example,  $\frac{N_{5,3}(9)}{9} > \frac{N_{5,3}(x)}{x}$  for any  $x \geq 12$ ) will not occur for parabolic or hyperbolic  $(r, q)$ . The reason is that, for parabolic or hyperbolic  $(r, q)$ , any two  $(r, q)$ -polycycles can be joined to form a bigger  $(r, q)$ -polycycle.

Furthermore, the above extends to some  $(R, q)$ -polycycles. For example, one such problem is to determine the  $(\{3, 4, 5, 6\}, 6)$ -polycycles (see Chapter 7) with the shortest perimeter for fixed  $p$ -vector. If  $3p_3 + 2p_4 + p_5 \leq 6$ , then the solution is shown in [An05] to be a kind of generalized spiral; previous work of Greinus [BBG03, Gre01] solved the  $(\{5, 6\}, 3)$ -polycycle case.

## 8.2 Non-extensible polycycles

Now we consider another natural notion of maximality for polycycles. An  $(r, q)$ -polycycle is called *non-extensible* if it is not a partial subgraph of any other  $(r, q)$ -polycycle, i.e., if an addition of any new  $r$ -gon removes it from the class of  $(r, q)$ -polycycles. It is clear that any tiling  $\{r, q\}$  is non-extensible, while all other non-extensible polycycles are helices. It is also clear that any 3-connected  $(r, 3)$ -polycycle is non-extensible.

Four exceptional non-extensible polycycles, depicted on Figure 8.3 are: vertex-split Octahedron, vertex-split Icosahedron and two infinite ones:  $P_2 \times P_{\mathbb{Z}} = Prism_{\infty}$  and  $Tr_{\mathbb{Z}} = APrism_{\infty}$  (see Section 4.2).

**Theorem 8.2.1** *All non-extensible  $(r, q)$ -polycycles are:*

- regular tilings  $\{r, q\}$ , ( $\{r, q\} - f$  in elliptic case),
- 4 exceptional examples in Figure 8.3,
- a continuum of infinite ones for any  $(r, q) \neq (3, 3), (3, 4), (4, 3)$ .

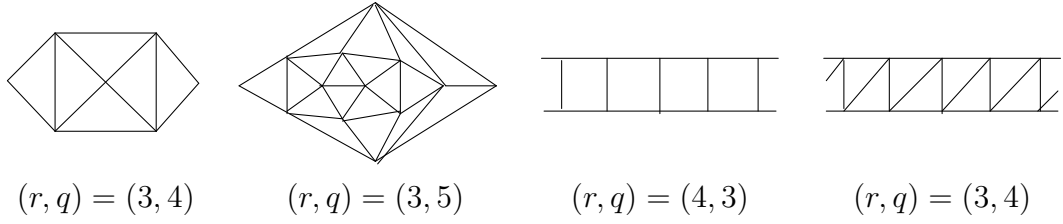


Figure 8.3: Exceptional non-extensible elliptic  $(r, q)$ -polycycles

**Proof.** The case  $(r, q) = (3, 3)$ ,  $(3, 4)$ ,  $(4, 3)$  follows immediately from the list of these polycycles given in Chapter 4. It is clear that doubly-infinite and non-periodic (at least in one direction) sequences of glued copies of the elementary polycycles  $b_2$  and  $e_6$  (from Figure 7.3) yield a continuum of infinite non-extensible  $(3, 5)$ -polycycles. By gluing the elementary  $(5, 3)$ -polycycles  $C_2$  (from Figure 7.2) and  $C'_2$  (obtained from  $C_2$  by rotation through  $\pi$ ), one obtains infinite non-extensible  $(5, 3)$ -polycycles. Clearly, there is a continuum of such. In Lemma 8.2.4, we will have a continuum of non-extensible  $(r, q)$ -polycycles for non-elliptic  $(r, q)$ .

For the parameters  $(r, q) = (3, 5)$ ,  $(5, 3)$ , in Lemma 8.2.3, we will prove that the vertex-split Icosahedron is unique such finite polycycle.  $\square$

**Lemma 8.2.2** *Any finite non-extensible  $(r, q)$ -polycycle is elliptic.*

**Proof.** The proof is based on curvature estimates. In fact, it is counting of vertex-face incidences plus using of Euler formula. We choose to use the curvature viewpoint (see Section 4.4) since it express nicely ellipticity.

Since the angle of a regular  $r$ -gon is equal to  $\frac{r-2}{r}\pi$  and the number of regular  $r$ -gons that meet at an internal vertex of the polycycle  $P$  is equal to  $q$ , the curvature of any internal vertex of the polycycle  $P$ , is equal to:

$$\omega = 2\pi - \frac{r-2}{r}q\pi.$$

Hence, the total curvature of the polycycle  $P$  is equal to:

$$\Omega = v_{int} \frac{2(r+q) - rq}{r} \pi.$$

If  $v_{int} = 0$ , i.e., an  $(r, q)$ -polycycle  $P$  is outerplanar, then the curvature  $\Omega$  is equal to zero for any parameters  $(r, q)$ . If  $v_{int} > 0$ , then the curvature  $\Omega$  is positive, zero, or negative, depending on whether the parameters  $(r, q)$  are elliptic, parabolic, or hyperbolic, respectively.

Any internal edge of a polycycle  $P$  belongs to exactly two  $r$ -gons, while any boundary edge belongs to only one  $r$ -gon. Therefore, the following equality holds:

$$rp_r = 2e_{int} + k,$$

where, again,  $e_{int}$  is the number of non-boundary edges of the polycycle  $P$  and  $k$  is the number of boundary edges. On the other hand, since the number of boundary vertices and the number of boundary edges of  $P$  are equal to the same number  $k$  (the perimeter

of the polycycle), these two numbers in the Euler formula cancel out, and a condensed version of this formula reads as:

$$v_{int} - e_{int} + p_r = 1.$$

From the last two formulas, one obtains:

$$(r - 2)p_r = 2v_{int} + (k - 2).$$

Now, let us calculate the sum of plane angles of the polycycle  $P$ . We do this in two different ways: (i) we first calculate the sum of angles in separate  $r$ -gons and then sum up over all  $r$ -gons and (ii) we first calculate the sum of angles at separate vertices and then sum up over all vertices, both boundary and internal. As a result, one obtains the equality:

$$p_r(r - 2)\pi = \sum_{i=1}^k \varphi_i + v_{int} \frac{r - 2}{r} q\pi,$$

where  $\varphi_i$  denotes the total angle at the  $i$ -th boundary vertex of  $P$ . Combining this formula with the preceding one, yields:

$$v_{int}(2\pi - \frac{r - 2}{r} q\pi) = \sum_{i=1}^k \varphi_i - (k - 2)\pi. \quad (8.1)$$

This formula is sometimes called Gauss-Bonnet formula (see [Ale50]). Expressed differently, Euler formula  $v - e + f = 2$  is for plane graphs with no boundaries but it can be extended to plane graphs with boundaries.

Let  $k_j$  be the number of vertices of degree  $j$  (where  $j = 2, 3, \dots, q - 1, q$ ) on the boundary of  $P$  and  $k$  be the total number of vertices of the boundary circuit of  $P$ , i.e., its perimeter. Then it holds:

$$k = k_2 + k_3 + \dots + k_{q-1} + k_q. \quad (8.2)$$

Let us calculate the sum  $\sum_{i=1}^k \varphi_i - (k - 2)\pi$  on the right-hand side of equality (8.1) for a finite polycycle  $P$  considered as a geodesic  $k$ -gon. Since it holds:

$$\sum_{i=1}^k \varphi_i = (1k_2 + 2k_3 + \dots + (q - 2)k_{q-1} + (q - 1)k_q) \frac{r - 2}{r} \pi,$$

by formula (8.2), one obtains the equality:

$$\begin{aligned} \sum_{i=1}^k \varphi_i - (k - 2)\pi = & \left( \left(1 \frac{r-2}{r} - 1\right)k_2 + \left(2 \frac{r-2}{r} - 1\right)k_3 + \dots \right. \\ & \left. + \left((q - 2) \frac{r-2}{r} - 1\right)k_{q-1} + \left((q - 1) \frac{r-2}{r} - 1\right)k_q \right) \pi + 2\pi. \end{aligned} \quad (8.3)$$

Consider a particular case of a finite polycycle  $P$  in which each vertex has degree  $q$ . In this case,  $2e = qn$ , where  $n$  is the total number of vertices and  $e$  is the total number of edges of  $P$ ; in view of the equality  $2e = rp_r + k$ , one can rewrite the Euler formula  $n - e + p_r = 1$  as follows:

$$n \frac{2(q + r) - qr}{2r} = 1 + \frac{k}{r}.$$

Hence,  $2(q+r) - qr > 0$ , i.e., the parameters  $(r, q)$  are elliptic. For any of the five elliptic pairs  $(r, q) = (3, 3), (3, 4), (3, 5), (4, 3), (5, 3)$ , we directly verify that the equality  $k = r$  holds and that  $P$  is, in fact, the surface of a Platonic body without one face.

Assume now that there exists a vertex of degree different from  $q$ . By Theorem 4.3.3, there are at least two such vertices.

Suppose that the parameters  $(r, q)$  are parabolic or hyperbolic, i.e., the inequality  $qr - 2(q+r) \geq 0$  holds. Then, the following estimate is valid for the coefficient of  $k_q$  in Equation (8.3):

$$(q-1)\frac{r-2}{r} - 1 = \frac{qr - 2(q+r)}{r} + \frac{2}{r} \geq \frac{2}{r}.$$

By Corollary 4.3.5, the total number of vertices on the boundary must be greater than  $r$ . Any two vertices of degree less than  $q$  should be separated by at least  $r-1$  vertices of degree  $q$ ; otherwise, the polycycle  $P$  would be extensible.

From the aforesaid and condition  $r \geq 3$ , it follows:

$$k_q \geq (r-1) \sum_{j=2}^{q-1} k_j \geq 2 \sum_{j=2}^{q-1} k_j.$$

Therefore, by (3), the quantity  $\sum_{i=1}^k \varphi_i - (k-2)\pi$ , calculated for the polycycle  $P$ , follows the bound:

$$\begin{aligned} \sum_{i=1}^k \varphi_i - (k-2)\pi \geq & \left( \left(1\frac{r-2}{r} - 1 + 2\frac{2}{r}\right)k_2 + \left(2\frac{r-2}{r} - 1 + 2\frac{2}{r}\right)k_3 + \dots \right. \\ & \left. + ((q-2)\frac{r-2}{r} - 1 + 2\frac{2}{r})k_{q-1} \right)\pi + 2\pi. \end{aligned} \quad (8.4)$$

The coefficient of  $k_j$  on the right-hand side of Inequality (8.4) increases as the index  $j$  increases. Since the least coefficient (that of  $k_2$ ) is positive, all the other coefficients of  $k_j$  are also positive. The values of  $k_j$  themselves are non-negative (and there even exists one positive  $k_j$  because there are vertices on the boundary of  $P$  whose degree is less than  $q$ ). Hence, it holds:

$$\sum_{i=1}^k \varphi_i - (k-2)\pi \geq 2\pi.$$

The positivity of the right-hand side of Inequality (8.4) implies the positivity of the left-hand side. Thus, in view of Equation (8.1), the curvature  $\Omega$  of the geodesic  $k$ -gon is positive. The resulting inequality  $2(r+q) - qr > 0$  contradicts the assumption made. Hence, a finite non-extensible polycycle cannot have parabolic or hyperbolic parameters  $(r, q)$ ; these parameters are elliptic.  $\square$

**Lemma 8.2.3** ([DSS06]) *All finite elliptic non-extensible  $(r, q)$ -polycycles are two vertex-splittings (of Octahedron and Icosahedron; see first two in Figure 8.3) and five Platonic  $\{r, q\}$  (with a face deleted).*

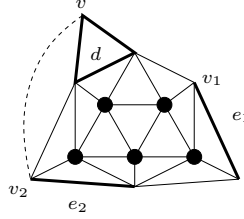
**Proof.** The case of  $(3, 3)$ -,  $(3, 4)$ - and  $(4, 3)$ -polycycles is resolved by using the classification of such polycycles in Section 4.2. Consider now a  $(r, q)$ -polycycle  $P$  with  $(r, q) = (3, 5)$  or  $(5, 3)$ . Then we can use the classification of the elementary  $(r, q)$ -polycycles given in Figure 7.2 and 7.3. Consider now its elementary components and the major skeleton  $Maj(P)$  formed by them with two components being adjacent if and only if they are adjacent on an open edge. Clearly,  $Maj(P)$  is a plane graph. But, by Theorem 8.0.1, it

is also a tree. So, either  $Maj(P)$  is reduced to a point, or  $Maj(P)$  has a vertex of degree 1.

Consider now the case  $(r, q) = (5, 3)$ . It is easy to see that the only finite elementary  $(5, 3)$ -polycycle, which is non-extensible, is  $A_1 = \{5, 3\} - f$ . Assume now that  $Maj(P)$  has a vertex of degree 1. Then, the elementary polycycle corresponding to this vertex is different from  $A_i$ . It is easy to see that for all other finite elementary  $(5, 3)$ -polycycles, one can extend, i.e., add one more face.

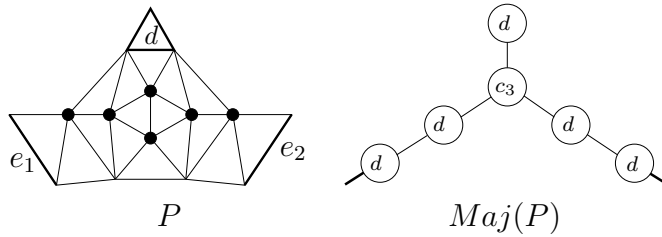
Consider now the case  $(r, q) = (3, 5)$  and take a non-extensible  $(3, 5)$ -polycycle  $P$ . The only finite elementary non-extensible  $(3, 5)$ -polycycle is  $a_1 = \{3, 5\} - f$ . Assume now that  $P$  is different from  $a_1$ , then it has more than one elementary component. So, the major skeleton  $Maj(P)$  has vertices of degree 1.

It is easy to see that all  $e_i$ ,  $b_i$  and  $c_i$  cannot be a vertex of degree 1 in  $Maj(P)$  since otherwise there will be an open edge on which one can add at least a 3-gon. So,  $d$  and  $a_3$  are the only possibilities for vertices of degree 1 in  $Maj(P)$ . If  $a_3$  occurs, then  $P$  is reduced to  $d + a_3$  as expected. So, let us assume that  $d$  occurs as vertices of degree 1. If  $d$  is adjacent to the elementary polycycle  $P_{el}$ , then the open edge to which  $d$  is incident, should have both vertices of degree 4 since, otherwise, one can add another 3-gon to  $d$ . The only elementary  $(3, 5)$ -polycycles having two vertices of degree 4 in succession are  $a_3$ ,  $c_2$  and  $c_3$ . If  $a_3$  occurs then we are done. The following diagram shows, up to symmetry, why  $c_2$  is impossible:



It is conceivable that one can add polycycle on the open edge  $e_1$  to forbid the extension by an edge  $v - v_1$ . But it is not possible to add a polycycle on  $e_2$ ; so, we are always able to add the edge  $v - v_2$  and  $P$  is extensible.

If  $c_3$  occurs, then we have the following diagram:



Since the polycycle  $P$  is non-extensible, there are some polycycles incident to the edges  $e_1$  and  $e_2$ . So, we have two paths starting from  $d$ . Since  $Maj(P)$  is a finite tree, those two paths will eventually terminate on a vertex of degree 1, which, by the above analysis, has to be another  $d$ . Furthermore, the elementary  $(3, 5)$ -polycycle preceding it, has to be  $c_3$ . So, again we have two paths, one of them new. This argument does not terminate. We do not find a cycle in  $Maj(P)$  since it is a tree and so we proved that  $P$  is infinite. This is impossible by the hypothesis and so, the only possibility is  $d + a_3$ .  $\square$

**Lemma 8.2.4** *For non-elliptic  $(r, q)$ , there is a continuum of non-extensible  $(r, q)$ -polycycles.*

**Proof.** We consider infinite non-extensible polycycles obtained from  $\{r, q\}$  by deleting certain non-adjacent  $r$ -gons followed by taking the universal cover. If we delete a countable number of  $r$ -gons using non-periodic sequences of deleted  $r$ -gons, then (due to an ambiguous choice of the deleted  $r$ -gons at each step) we obtain a continuum of different polycycles. Consider two non-congruent sequences  $S_1$  and  $S_2$  of  $r$ -gons in  $\{r, q\}$ , the  $(r, q)_{gen}$ -polycycles  $P_1 = \{r, q\} - S_1$  and  $P_2 = \{r, q\} - S_2$  are not isomorphic, their universal covers  $\tilde{P}_1$  and  $\tilde{P}_2$  are non-extensible  $(r, q)$ -polycycles, whose image in  $\{r, q\}$  by the cell-homomorphism (see Theorem 4.3.1) is  $P_1$  and  $P_2$ . Therefore,  $P_1$  and  $P_2$  are not isomorphic.  $\square$

Finally, consider  $(r, q)$ -polycycles, such that any interior point of any interior face has degree 1 of the cell-homomorphism onto  $\{r, q\}$ . The number of such polycycles, which are not extensible without losing this property, is equal to 0 for  $(p, q) = (3, 3), (3, 4)$  and equal to 1 for  $(p, q) = (4, 3)$  (it is  $P_2 \times P_5$ ). This number is finite for  $(p, q) = (5, 3), (3, 5)$  and infinite, otherwise. The finiteness of this number for the parameters  $(r, q) = (5, 3)$  and  $(3, 5)$  follows from the fact that the number of 5-gons and 3-gons must be no greater than 12 and 20, respectively.

### 8.3 2-embeddable polycycles

We shortly presented 2-embedding of polycycles just as an application of elementary polycycles. 2-embedding of graphs is the main subject of the book [DGS04]. Let us only mention enumeration of 2-embeddable  $(\{a, 6\}, 3)$ -spheres ( $a = 3, 4, 5$ ). There are 1, 5, 5 such graphs for  $a = 3, 4, 5$  (see [DeDuSh05, MaSh07]).

Given a set  $S$ , the *Hamming distance* on  $|S|$ -hypercube  $\{0, 1\}^{|S|}$  is defined by  $d(x, y) = |\{i \in S : x_i \neq y_i\}|$ . Given two vertices  $u, v$  of a graph  $G$ , the *path-distance*  $d_G(u, v)$  is the minimal number of edges needed to connect  $u$  to  $v$ .

A graph  $G$  is said to be *2-embeddable* (*embeddable*, for short) if there exist a set  $S$  and a function

$$\begin{aligned} \psi : V(G) &\rightarrow \{0, 1\}^{|S|} \\ v &\mapsto \psi(v) \end{aligned}$$

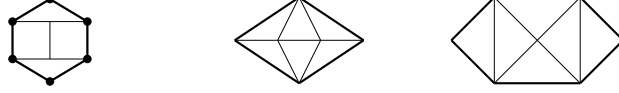
such that for all vertices  $v, v'$  of  $G$ , one has  $d(\psi(v), \psi(v')) = 2d_G(v, v')$  with  $d_G$  being the path-distance on  $G$ . For more informations on this subject, see [DeLa97, DGS04] and reference therein. For finite graphs, an efficient polynomial time algorithm for recognizing 2-embeddable plane graphs is given in [DeSh96] (see an implementation in [Dut2]).

Given a plane graph  $G$ , an *alternating zone* is a sequence  $(e_i)$  of edges such that  $e_i$  and  $e_{i+1}$  belong to the same face  $F_i$ . If  $F_i$  has an even number of vertices, then we require  $e_i$  and  $e_{i+1}$  to be on opposite side in  $F_i$ . If  $F_i$  has an odd number of faces then  $e_i$  and  $e_{i+1}$  are again in opposition but then we have two choices denoted, up to rotation of the plane,  $+$  and  $-$ . We require that the choices  $+$  and  $-$  are alternating. The final edges of the zone (incident to exterior faces) are called the *ends* of the zone. If the zone is not self-intersecting, then, after removal of the edges of the zone, one obtains two graphs  $G_1$  and  $G_2$ . If each shortest path in  $G$  between two vertices of  $G_i$  for a fixed  $i = 1, 2$  consists only of edges in this subgraph  $G_i$ , then we say that the zone realizes a *convex cut* of the given  $(r, q)$ -polycycle. If every alternating zone realizes a convex cut, then the graph is 2-embeddable (see [CDG97] for a proof).

A  $(r, q)$ -graph is a plane graph such that all interior faces have at least  $r$  edges and all interior vertices have degree at least  $q$ . In [PSC90] it is proved that  $(4, 4)$ -graphs are 2-embeddable and it is proved in [CDV06] that  $(6, 3)$ - and  $(3, 6)$ -graphs are 2-embeddable. This implies that all  $(r, q)$ -polycycles with parabolic or hyperbolic  $(r, q)$  are 2-embeddable.

This and a check for elliptic  $(r, q)$  in Section 4.2 gives the following:

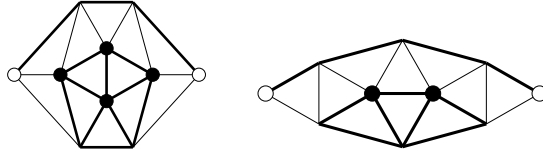
**Theorem 8.3.1** *For  $(r, q) \neq (5, 3), (3, 5)$ , only three finite  $(r, q)$ -polycycles are not 2-embeddable:*



So, it remains to solve the 2-embedding problem only for  $(r, q) = (3, 5)$  and  $(5, 3)$ . If an elementary polycycle  $P$  appears in the decomposition of a polycycle  $P'$ , then  $P$  is an isometric subgraph of  $P'$ .

**Theorem 8.3.2** ([DeSt02a]) *A  $(3, 5)$ -polycycle different from Icosahedron  $\{3, 5\}$  and Icosahedron with one vertex removed  $\{3, 5\} - v$ , is 2-embeddable if and only if it does not contain, as an induced subgraph, any of  $(3, 5)$ -polycycles  $c_3$  and  $d + e_2 + d$  shown in Figure 8.4.*

**Proof.** The  $(3, 5)$ -polycycles  $c_3$  and  $d + e_2 + d$  are not 2-embeddable. So, some of their alternating zones do not define convex cuts:



The edge of induced graphs  $G_i$  defined at the beginning of this section are boldfaced. Between the vertices in white, there are two shortest paths, one outside of the subgraph. The two polycycles  $a_1 = \{3, 5\} - f$  and  $a_5 = \{3, 5\} - v$  are 2-embeddable. The two polycycles  $a_5 + d$  and  $d + a_5 + d$ , containing  $d + e_2 + d$ , are, on the other hand, not 2-embeddable. There are no other  $(3, 5)$ -polycycles containing  $a_5$  as an elementary summand. The polycycles  $a_2, a_3, a_4, b_2, b_3, c_1, c_2, c_3$  have at least one non 2-embeddable polycycle  $c_3$  amongst their isometric sub-polycycles. The polycycles  $e_i, i \geq 4, b_1$  and  $a_6$  contain an isometric non 2-embeddable sub-polycycle  $d + e_2 + d$ . By virtue of this, any  $(3, 5)$ -polycycle containing any of these polycycles as an elementary summand, is not 2-embeddable.

It remains to investigate the  $(3, 5)$ -polycycles with elementary summands  $c_4, d, e_1, e_2, e_3$ . We assume that  $c_3$  and  $d + e_2 + d$  do not appear as sub-polycycle and we will prove that their alternating zone define convex cuts.

Let us take an alternating zone. The lateral sides of a 3-gon lie interior to the zone; only the extreme left and extreme right of them are the end of the zone; the base of a 3-gon lie on the boundary of the zone. Suppose that the base of a 3-gon belongs to the kernel. Then a polycycle  $e_2$ , that has this base as kernel, is a sub-polycycle of the given  $(3, 5)$ -polycycle. There is only one edge of  $e_2$ , both ends of which have degree 3, to which a 3-gon  $d$  can be added (the polycycle  $d + e_2 + d$  is forbidden); another such edge of  $e_2$  is always an end of the zone. If the boundary of the zone does not contain two bases in succession belonging to the kernel, then another such base can only occur on the boundary of the zone at its other end. Of all the vertices on the boundaries of the zone

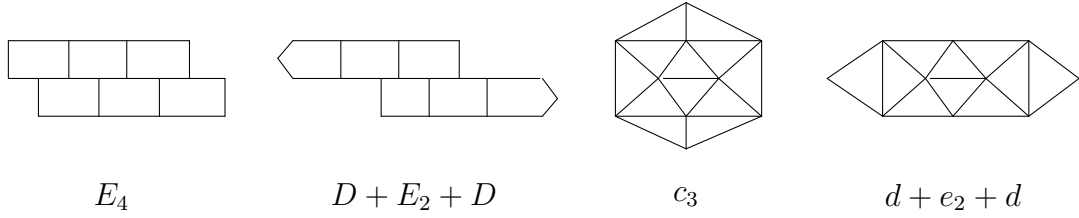
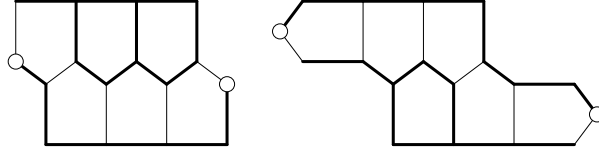


Figure 8.4: Forbidden subgraphs of non-embeddable  $(5, 3)$ - and  $(3, 5)$ -polycycles

not belonging to these bases in the kernel, at least every other one lies on the boundary of the surrounding  $(3, 5)$ -polycycle. By this, the zone defines a convex cut. But if two bases in succession on the boundary of the zone belong to the kernel, then the zone has 8 edges in all; both its ends are edges of an elementary polycycle  $e_3$  with ends of degree 3. They define convex cuts.  $\square$

**Theorem 8.3.3** ([DeSt00b]) *A  $(5, 3)$ -polycycle different from Dodecahedron  $\{5, 3\}$  is 2-embeddable if and only if it does not contain any of  $(5, 3)$ -polycycles  $E_4$  and  $D + E_2 + D$  (see Figure 8.4) as an induced subgraph.*

**Proof.** The  $(5, 3)$ -polycycles  $E_4$  and  $D + E_2 + D$  are non 2-embeddable. So, some of their alternating zone do not define convex cuts:



The  $(5, 3)$ -polycycle  $A_1$  is 2-embeddable. The elementary  $(5, 3)$ -polycycles  $A_2, A_3, A_4, A_5, A_6 = E_{\mathbb{Z}}, B_1 = E_{\mathbb{N}}, B_2, B_3, C_1, C_2$  contain  $E_4$  as induced subgraph and so, they are not 2-embeddable.

Consider now a  $(5, 3)$ -polycycle, different from  $A_1$ , which does not contain  $E_4$  and  $D + E_2 + D$  as partial subgraph. From the above we know that its possible elementary components are  $D, E_2, E_3, C_3$ . Take an alternating zone  $Z$  passing through elementary components  $\dots, EP_i, \dots$ . We know that if  $E_2$  appears in this list, then it is an end of the sequence, since  $D + E_2 + D$  is forbidden. Now, looking at the zone itself, one sees that  $E_3$  and  $C_3$  also have to be at the end. Therefore, we have only  $D$  in the middle of the sequence  $EP_i$ . But  $D$  can be glued to only two other elementary  $(r, q)$ -polycycles. Then one checks that the alternating zones are convex (this is long and cumbersome).  $\square$

What we considered above was 2-embedding into  $\{0, 1\}^{|S|}$ . If the graph  $G$  is finite, then  $S$  is finite. If  $G$  is infinite, one can consider embedding of  $G$  into  $\mathbb{Z}^{|S|}$  with the distance  $d(x, y) = \sum_{i \in S} |x_i - y_i|$ . Any 2-embedding into  $\mathbb{Z}^{|S|}$  gives a 2-embedding into  $\{0, 1\}^{|T|}$  for some  $T$ . But we might be able to embed into  $\mathbb{Z}^{|S|}$  with finite  $S$  even when  $G$  is infinite. This actually happens for the parabolic tilings  $\{4, 4\} = \mathbb{Z}^2$ ,  $\{3, 6\}$ ,  $\{6, 3\}$  (both are 2-embeddable into  $\mathbb{Z}^3$ ) and for infinite  $(4, 4)$ -,  $(3, 6)$ -,  $(6, 3)$ -graphs, but not for the hyperbolic tilings. But there are infinite parabolic  $(r, q)$ -polycycles which are 2-embeddable into  $\mathbb{Z}^{|S|}$  only for infinite  $S$ .

